

Nuclear Physics from Lattice QCD

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Abstract

We review recent progress toward establishing lattice Quantum Chromodynamics as a predictive calculational framework for nuclear physics. A survey of the current techniques that are used to extract low-energy hadronic scattering amplitudes and interactions is followed by a review of recent two-body and few-body calculations by the NPLQCD collaboration and others. An outline of the nuclear physics that is expected to be accomplished with Lattice QCD in the next decade, along with estimates of the required computational resources, is presented.

1 Introduction

It has been known for the past four decades that Quantum Chromodynamics (QCD), together with the electroweak interactions, underlies all of nuclear physics, from the s-wave nucleon-nucleon scattering lengths to the mechanism of synthesis of heavy elements in stars. Soon after the discovery of QCD it became apparent that the complexities of the theory at strong coupling would hinder analytic progress in understanding the properties of the simplest hadrons, let alone the simplest features of the nuclear forces. Wilson pointed the way to eventual direct quantitative confirmation of the origins of nuclear physics by formulating Lattice QCD [1], a regularization and non-perturbative definition of QCD that is suitable for the intensive computational demands of solving QCD in the infrared.

Only in the last five years or so has Lattice QCD emerged from a long period of research and development —where only qualitative agreement between calculations and experiments could be claimed— to the present, where precise predictions for hadronic quantities are being made. In particular, presently, fully-dynamical calculations with near-exact chiral symmetry at finite lattice-spacing have become standard, with lattice volumes of spatial extent $L \gtrsim 2.5$ fm and with lattice spacings in the range $b \lesssim 0.12$ fm. Very recently, preliminary calculations at the physical quark masses have been carried out. However, it is still the norm that the light-quark masses, m_q , are larger than those of nature, with typical pion masses $m_\pi \sim 300$ MeV. It is expected that in the next five years, calculations at the physical light-quark masses, $m_\pi \sim 140$ MeV, in large volumes, $L \gtrsim 6$ fm, and at small lattice spacings, $b \lesssim 0.06$ fm will become commonplace.

Nuclear physics is a vast, rich field, whose phenomenology has been explored for decades through intense experimental and theoretical effort. However, there is still little understanding of the connection

to QCD and the basic building blocks of nature, quarks and gluons. For instance, as a first “benchmarking” step, Lattice QCD should post-dict the large nucleon-nucleon scattering lengths and the existence of the deuteron, the simplest nucleus. The connection between QCD and nuclear physics will be firmly established with Lattice QCD, and will allow for an exploration of how nuclei and nuclear interactions depend upon the fundamental parameters of nature. In particular, it is believed that an understanding of the fine-tunings that permeate nuclear physics will finally be translated into fine-tunings of the light-quark masses. While these issues are of great interest, and it is important to recover what is known experimentally to high precision, these goals are not the main objective of the Lattice QCD effort in nuclear physics. The primary reason for investing resources in this area is to be able to calculate physical quantities of importance that cannot be accessed experimentally, or which can be measured with only limited precision in the laboratory. Two important examples of how Lattice QCD calculations can impact nuclear physics are in the structure of nuclei and in the behavior of hadronic matter at densities beyond that of nuclear matter.

Refined many-body techniques for studying the structure of nuclei, such as Greens function Monte-Carlo (GFMC) [2], already exist. This method has led to calculations of the ground states and excited states of light nuclei, with atomic number $A \lesssim 14$. Using only the modern nucleon-nucleon (NN) potentials that reproduce all scattering data below inelastic thresholds with $\chi^2/dof \sim 1$, such as AV_{18} [3], these models fail to recover the observed structure of light nuclei. However, the inclusion of a three-nucleon interaction greatly improves the predicted structure of nuclei [2]. Lattice QCD will be able to calculate the interactions of multiple nucleons, bound or unbound, in the same way that it can be used to determine the two-body scattering parameters. For instance, a calculation of the three-neutron interactions will be possible.

One of the great challenges facing nuclear physics is to determine the behavior of hadronic matter at densities away from that of nuclear matter, such as those that occur in the interior of neutron stars [4]. There are a number of possibilities for the composition of the hadronic matter at the center of a neutron star. One possibility is that it is composed of neutrons and protons. Another possibility is that it is composed of neutrons, protons and a kaon condensate, and a third possibility is that it is composed of neutrons, protons and Σ^- 's. At present, all of these compositions (and other more exotic scenarios) are possible theoretically, and not excluded experimentally or observationally. On the theoretical side, the main uncertainty in establishing the composition of hadronic phases, and hence the equation of state, is the interactions between the strange hadrons, such as the kaon and Σ^- , and the protons and neutrons. These interactions are poorly known experimentally due to the short lifetime of the strange hadrons, however Lattice QCD promises to reliably calculate these interactions from QCD with quantifiable uncertainties. Indeed lattice QCD calculations will provide the best determinations of hyperon-nucleon and kaon-nucleon scattering amplitudes and hence will play a crucial role in determining the role of hyperons and strange mesons in neutron stars.

Lattice QCD is a technique in which Euclidean space correlation functions are calculated by a Monte-Carlo evaluation of the Euclidean space path integral [1]. The calculations are performed in Euclidean space so that field configurations that have a large action are exponentially suppressed. This is in contrast with Minkowski space in which large action contributions result in a complex phase which will average to an exponentially small contribution with nearby configurations. In this approach, space-time is discretized with the quarks residing on the lattice sites, and the gluon fields residing on the links between lattice sites. The lattice spacing, b , the distance between adjacent lattice sites, is required to be much smaller than the characteristic hadronic length scale of the system under study. The effects of a finite lattice spacing can be systematically removed by combining calculations of correlation functions at several lattice spacings with the low-energy effective field theory (EFT) which explicitly includes the discretization effects. This type of EFT is somewhat more complicated than its continuum counterpart as it must reproduce matrix elements of the Symanzik action constructed with higher dimension operators induced by the discretization [5]. While the action lacks Lorentz invariance and

rotational symmetry, it is constrained by hypercubic symmetry. As computers have finite memory and performance, the lattice volumes are finite in all four space-time directions. Generally, periodic boundary conditions (BC's) are imposed on the fields in the space-directions (a three-dimensional torus), while (anti-)periodic BC's are imposed on the (quark) gauge fields in the time-direction, which in many cases is much larger than the space-directions (in order to approach the zero-temperature limit).

For the calculations we will be discussing in this review, the lattice volumes are large compared with the Compton wavelength of the pion, and deviations of single-particle properties from their infinite volume values are exponentially small, generically $\sim e^{-m_\pi L}$. These finite-volume effects may be removed by finite-volume EFT. Perhaps the most important “economic” feature of Lattice QCD calculations is that the computational resources required to perform lattice calculations increase with decreasing quark mass, and presently, no calculations exist at the physical quark masses, $m_\pi \sim 140$ MeV, that have $m_\pi L \gg 1$. It remains the case that lattice calculations are performed at unphysical values of the quark masses, and the light quark mass dependence of the observable of interest, which can be determined perturbatively in the low-energy EFTs, is used to extrapolate to the physical light quark masses. Therefore, the practical situation with current Lattice QCD calculations is that they are performed at finite lattice spacing, within finite volumes and at unphysical quark masses. The appropriate EFT (e.g. chiral perturbation theory (χ -PT), heavy-baryon- χ -PT (HB χ -PT)) is then used to extrapolate to the infinite volume, continuum limit of QCD where physical predictions can be made.

2 Lattice QCD Technology

Quantum Chromodynamics (QCD) can be defined non-perturbatively as the continuum limit of a Lattice gauge theory. This approach provides both an ultraviolet regulator of the continuum field theory and admits numerical evaluation of the functional integrals required for calculating physical observables. In the continuum, the QCD path integral is ¹

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}A_\mu \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-\int d^4x \mathcal{L}_{\text{QCD}}} \\ \mathcal{L}_{\text{QCD}} &= \sum_f \bar{\psi}_f [D_\mu \gamma_\mu + m_f] \psi_f + \frac{1}{4} \sum_a G_{\mu\nu}^a G^{a\mu\nu} \quad , \end{aligned} \quad (1)$$

where \mathcal{L}_{QCD} is the QCD Lagrange density, A_μ is the QCD gauge field (describing the gluons), $G_{\mu\nu}^a$ is the gauge field strength, m_f is the quark mass, and $\bar{\psi}_f, \psi_f$ are the fermion fields representing the quark flavors. D_μ is the covariant derivative which ensures gauge invariance and γ_μ are the Dirac-matrices. Explicitly, the covariant derivative acting on a quark field is given by

$$D_\mu \psi(x) = \partial_\mu \psi(x) + ig_s A_\mu(x) \psi(x) \quad , \quad A_\mu(x) = T^a A_\mu^a(x) \quad , \quad (2)$$

where $T^a = \lambda^a/2$ with the λ^a being the Gell-Mann matrices. The strong coupling g_s appearing in eq. (2) is related to the strong fine-structure constant, α_s , via $\alpha_s = g_s^2/(4\pi)$. The field strength tensor is defined in terms of the gluon field through

$$G_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + ig_s [A_\mu(x), A_\nu(x)] \quad , \quad G_{\mu\nu}(x) = G_{\mu\nu}^a(x) T^a \quad , \quad (3)$$

Observables (physical quantities) in this theory can be calculated from correlation functions of operators \mathcal{O} that are functions of the quantum fields (quarks and gluons).

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}A_\mu \mathcal{D}\bar{\psi} \mathcal{D}\psi \mathcal{O} e^{-\int d^4x \mathcal{L}_{\text{QCD}}} \quad . \quad (4)$$

¹A very nice introduction to Lattice QCD can be found in Ref. [6].

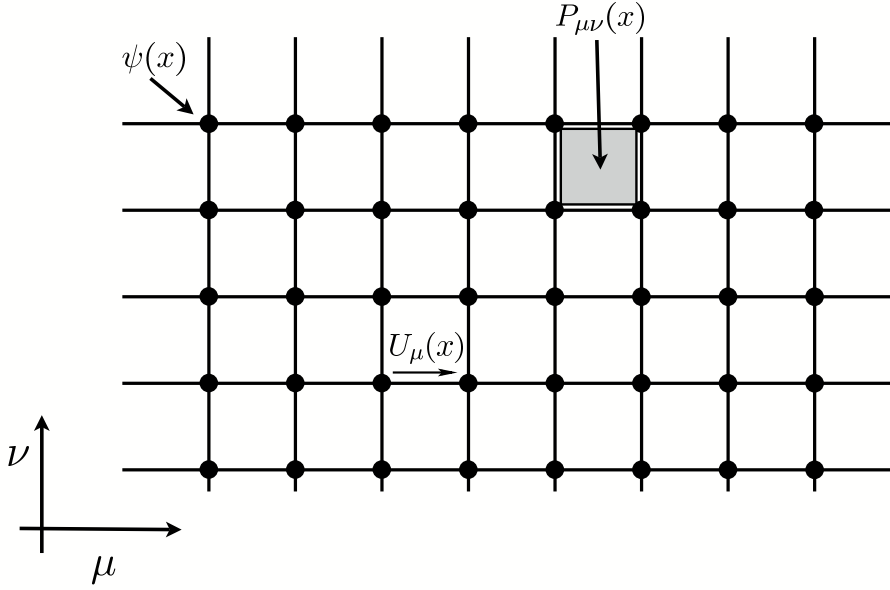


Figure 1: A two dimensional slice of the four dimensional space-time lattice. μ and ν denote unit-vectors in the indicated directions. $\psi(x)$ denotes a fermion-field at the lattice-site x , $U_\mu(x)$ denotes the gauge link from the lattice-site x to the site $x + b\mu$, and $P_{\mu\nu}(x)$ denotes the 1×1 Wilson plaquette centered at $x + b\mu/2 + b\nu/2$.

The path integral can be rigorously defined on a discrete space-time. In order to preserve gauge invariance the gauge fields are discretized as special unitary matrices, in the group $SU(3)$, on the links of the lattice (see Figure 1). The discrete gauge action is the sum over all plaquettes $P_{\mu\nu}(x)$ which are the product of the links $U_\mu(x) = \exp\left(i \int_x^{x+\hat{\mu}} dx' A_\mu(x')\right)$ around the elementary plaquettes of the lattice,

$$S_g(U) = \beta \sum_{x\mu\nu} \left(1 - \frac{1}{3} \text{Re Tr } P_{\mu\nu}(x)\right) , \quad (5)$$

with

$$P_{\mu\nu} = U_\mu(x)U_\nu(x + \hat{\mu})U_\mu^\dagger(x + \hat{\mu} + \hat{\nu})U_\nu^\dagger(x) . \quad (6)$$

β is the lattice gauge coupling that is related to the strong coupling via $\beta = 2N_C/g_s^2$ where N_C is the number of colors. Taking the naive continuum limit, this action becomes the familiar continuum gauge action, $-\int d^4x \frac{1}{4} (G_{\mu\nu}^a(x))^2$. The action in Eq. 5 is the well known Wilson gauge [1] action, and while this discretization is not unique, it is the simplest. It can be modified by adding larger loops with coefficients appropriately chosen to achieve better convergence to the continuum, which is the ultimate goal of the calculation.

Inclusion of the quarks (fermions), which are defined on the vertices of the lattice, is a challenging problem. A naive discretization of a single continuum fermion field introduces sixteen light lattice fermion flavors in the four dimensions. In QCD only three light quarks (up, down and strange) and three heavy quarks (top, bottom and charm) are needed. The doublers, i.e. the additional light lattice fermion degrees of freedom, can be avoided by several ingenious formulations of lattice fermions. Wilson fermions, which were introduced first [1], eliminate the doublers by adding irrelevant dimension five operators in the action that lift the masses of the doublers, leaving only one light fermion in the spectrum. However, this explicitly breaks chiral symmetry and introduces lattice artifacts that scale as $O(b)$. The Wilson action can be improved by the addition of one dimension-5 bilinear operator, $\mathcal{O}_{SW} = \bar{\psi} \sigma^{\mu\nu} G_{\mu\nu} \psi$, the Sheikholeslami-Wohlert term [7], with a coefficient, C_{SW} , that can be tuned so that the lattice artifacts are parametrically reduced to scale as $O(b^2)$. In addition, the lattice spacing artifacts can be reduced to $O(b^2)$ by the addition of a twisted-mass term to the action [8]. The isospin violation that the twisted-mass term introduces into the action can be removed using chiral perturbation theory. Kogut-Susskind fermions [9] (staggered fermions) provide another way to remove some of the doublers and re-interpret the remaining four as four degenerate flavors. In this approach a $U(1)$ chiral symmetry still remains unbroken and lattice artifacts scale as $O(b^2)$. Kogut-Susskind fermions become problematic when the required number of flavors is not a multiple of four (as is the case for QCD). In addition, the broken flavor and chiral symmetries introduce large lattice artifacts, although they scale as $O(b^2)$. Finally, the so called domain wall fermions [10, 11, 12] and overlap fermions [13, 14] are fermionic actions that both preserve a lattice chiral symmetry at finite lattice spacing (they satisfy the Ginsparg-Wilson relation [15] $\gamma_5 D + D \gamma_5 = b D \gamma_5 D$) and are doubler free. Unfortunately, such formulations are computationally significantly more expensive. It should also be stated that other actions are being explored that approximately satisfy the Ginsparg-Wilson relation, for instance the fixed-point action [16], or the chirally-improved action, e.g. Ref. [17, 18]. In all cases the lattice fermion action is of the form

$$S_f = \bar{\psi} D(U) \psi \quad (7)$$

where ψ is the fermion “vector” and $D(U)$ is a sparse matrix² acting on the fermion vector, that depends on the gauge field U . As an example of the form of S_f for a lattice action, its explicit form for the naive Wilson action is

$$S_f^{\text{Wilson}} = \frac{1}{2b} \sum_x \bar{\psi}(x) \gamma_\mu [U_\mu(x) \psi(x + b\mu) - U_\mu^\dagger(x - b\mu) \psi(x - b\mu)] + m_f \sum_x \bar{\psi}(x) \psi(x) . \quad (8)$$

The partition function in the case of two quark flavors is

$$\begin{aligned} \mathcal{Z} &= \int \prod_{\mu, x} dU_\mu(x) \prod_x d\bar{\psi} d\psi e^{-S_g(U) - S_f(\bar{\psi}, \psi, U)} \\ &= \int \prod_{\mu, x} dU_\mu(x) \det(D(U)^\dagger D(U)) e^{-S_g(U)} . \end{aligned} \quad (9)$$

The integration over the quark fields, which are represented by Grassmann numbers, can be done exactly. In addition, the quark matrix $D(U)$ represents one flavor, however since $\det D(U)^\dagger = \det D(U)$, the determinant $\det(D(U)^\dagger D(U))$ represents two flavors. In the case of correlation functions, integrating out the quarks gives the following expression

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{\mu, x} dU_\mu(x) \mathcal{O}\left(\frac{1}{D(U)}, U\right) \det(D(U)^\dagger D(U)) e^{-S_g(U)} , \quad (10)$$

²In certain cases, such as with overlap fermions, the matrix is not sparse but has sparse like properties, i.e. the matrix vector multiplication is a computationally “cheap” operation.

where the quantities \mathcal{O} depend on the inverse of the quark matrix and possibly explicitly on the gauge fields. The above expressions are only valid in the case of two flavors of quarks (the up and the down) which both have the same mass, which is a good approximation to the low energy physics of QCD. A strange quark can be easily added by including $\det(D(U)^\dagger D(U))^{1/2}$ in the partition function.

The computation of Eq. (10) is the main numerical task faced in Lattice QCD calculations. The integral over the gauge fields in Eq. (10) is of extremely large dimensionality. Given that QCD has a fundamental length scale of ~ 1 fm (10^{-13} cm), calculations must be performed in lattice volumes that have a physical size much larger than 1 fm in order to control finite volume effects, and with lattice spacings much smaller than 1 fm in order to be close to the continuum limit. With moderate choices for the volume and the lattice spacing, a lattice volume of $\gtrsim 32^3 \times 256$ is currently practical. With the color and spin degrees of freedom, such calculations involve $\approx 10^9$ degrees of freedom. The only practical way that this type of computation can be done is by using Monte-Carlo integration. Fortunately, the combination of the quark determinant and the gauge action,

$$\mathcal{P}(U) = \frac{1}{Z} \det(D(U)^\dagger D(U)) e^{-S_g(U)}, \quad (11)$$

is a positive definite quantity which can be interpreted as a probability and hence importance sampling can be employed. The basic algorithm is to produce N gauge field configurations $\{U\}$ with probability distribution $\mathcal{P}(U)$ and then evaluate

$$\langle \mathcal{O} \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \mathcal{O}\left(\frac{1}{D(U_i)}, U_i\right). \quad (12)$$

At finite N , the estimate of \mathcal{O} is approximate, with an uncertainty that converges to zero as $\mathcal{O}(1/\sqrt{N})$. Both for the gauge field configuration generation and the evaluation of Eq. (12), the linear system of equations

$$D^\dagger(U)[m]D(U)[m]\chi = \phi, \quad (13)$$

needs to be solved where the dependence of the quark matrix on the quark mass m is made explicit. Since the quark matrix is sparse, iterative solvers such as conjugate gradient (CG) can be used. The condition number of the quark matrix is inversely proportional to the quark mass. Since the physical quark masses for the up and down quarks are quite small, the quark matrix has a large condition number. With current computer resources this linear system cannot be solved exactly at the physical quark mass. For that reason the calculation is performed at heavier quark masses and then extrapolated to the physical point. The vast majority of the computer time used in these calculations is devoted to the solution of this linear system both in the context of gauge field generation and in the later stage of the calculation of physical observables through Eq. (12).

Realistic lattice calculations require quark masses that result in pion masses below 400 MeV, allowing chiral EFT's to be used with some reliability. In addition, a dynamical strange quark is required in order to guarantee that the low energy constants of the EFT determined with lattice QCD match those of the physical theory. Although this task seems formidable, in the last several years there have been developments that make phenomenologically interesting calculations now possible.

The works that we will be reviewing involves the computation of correlation functions with fixed particle number, for instance, correlation functions with the quantum numbers of the deuteron, or the correlation functions with the quantum numbers of twelve charged kaons. As the number of particles increases, the complexity of forming the correlation function grows dramatically, due to the need for the quarks to satisfy the Pauli principle. An alternate way to describe systems with large numbers of baryons, for instance, is to introduce a baryon-number chemical potential into the partition function in Eq. (1). However, the evaluation of the partition function with such a chemical potential is complicated

by the fact that the measure of the integration is no longer positive definite, that is to say, it suffers from the well-known sign-problem. Incremental progress has been made in dealing with the sign-problem, and a conceptual break through will be required in order to calculate the properties of systems at high densities and low-temperatures. Naively it appears that there should be a direct connection between the sign-problem and the behavior of multi-baryon correlation functions. However, to date, little connection between the two approaches to the numerical evaluation of the properties of finite-density systems has been established. A recent review of the status of calculations at finite density using chemical potentials can be found in Ref. [19].

2.1 *Lattice Fermion Actions*

The emergence of fermions that respect chiral symmetry [10, 11, 12, 13, 14] on the lattice was one of the major recent developments in Lattice QCD. These formulations of lattice fermions allow for the reduction of the lattice spacing errors and approach the continuum limit in a smooth manner. However, the computational resources required to calculate with these fermions are an order of magnitude larger than any other variant of lattice fermions. In addition, the development of improved Kogut-Susskind fermion actions [20, 21] that significantly reduce the $O(b^2)$ errors, allowed for “cheap” inclusion of quark loop effects in the QCD correlation functions computed on the lattice. With this formulation, volumes with spatial extent as large as $L \sim 5.8$ fm are being used with light-quark masses as low as 1/20th of the strange quark mass depending on available computing resources. However the fact that Kogut-Susskind fermions represent four flavors of quarks complicates calculations when two or one flavors are needed. From the operational point of view the problem is solved by introducing the Kogut-Susskind determinant raised to the $n_f/4$ power (rooted) into the path integral, where n_f is the desired number of flavors. The non-integer power of the quark determinant introduces non-localities in the lattice action. It has been argued that the long distance physics that survives the continuum limit is not affected by such non-localities [22, 23, 24, 25, 26, 27]. In addition, at finite lattice spacing, the pathologies arising in the Kogut-Susskind fermion formulation can be dealt with in staggered χ -PT [23, 24, 28]. Although no rigorous proof exists, empirical evidence indicates that Kogut-Susskind fermions do describe the correct physics as long as the continuum limit is taken before the chiral limit [27]³. The results presented in this review that are based upon mixed-action calculations on the MILC lattice ensembles assumes that the continuum limit of such calculations is QCD.

Finally, significant simulation algorithm developments have been achieved that have sped up the gauge field generation by orders of magnitude. Developments in the integrators needed for the molecular dynamics [30] that form the core of the Hybrid Monte-Carlo algorithm [31, 32] are one important component of the improvements. A second important component of the new algorithms is preconditioned Hybrid Monte-Carlo [33, 34, 35] and rational hybrid Monte-Carlo (RHMC) [38] for calculations involving an odd number of flavors. Together with multiple time scales [36, 37] for evolving different parts of the molecular dynamics Hamiltonian, calculations close to or at the physical quark masses became possible for a variety of lattice fermion actions including Wilson, Kogut-Susskind and domain-wall. For a status review of the current dynamical simulation algorithms the reader is referred to [39]. The result of these algorithmic developments was that calculations with Wilson or improved Wilson fermions again became feasible. In addition dynamical simulations with domain wall fermions are also possible at relatively small additional “cost” compared to “cheap” fermion variants at the same physical parameters. The choice of the computational approach is made based on the resources each collaboration has available as well as the physics objectives.

³It should be noted that there are some members of the lattice community who believe that the rooted-staggered action is fundamentally flawed and its continuum limit does not correspond to QCD (for a summary of these arguments, see Ref. [29]). We disagree with these arguments, however we acknowledge that there is no proof that the continuum limit of the rooted-Kogut-Susskind action corresponds to QCD.

2.1.1 *Mixed Action Calculations*

The mixed-action calculations discussed in this review employed Kogut-Susskind fermions to represent the QCD vacuum polarization effects associated with the two light flavors (up/down quarks) and the somewhat heavier strange quark. This is done by using gauge configurations generated with the appropriate Kogut-Susskind fermion determinants incorporated into the probability distribution that enters the path integral. Since this part of the computation is separated from the calculation of correlation functions, gauge fields generated by other collaborations can be used. NPLQCD made use of a number of ensembles of gauge configurations generated by the MILC collaboration [40]. Domain wall fermions were used to describe all external (valence) quarks. Because of the chiral symmetry that domain wall fermions satisfy, all correlation functions satisfy chiral Ward identities, ensuring that the leading order (LO) chiral behavior is continuum-like. The small corrections appearing due to Kogut-Susskind fermions in the vacuum loops can be taken care of systematically in χ -PT [41, 42, 43]. Compared to calculations with Kogut-Susskind fermions in the valence sector, this formulation results in better control of the chiral behavior and possibly smaller discretization errors and also simplifies calculations with baryons. This approach was first introduced by the LHP collaboration for the study of nucleon structure [44, 45, 46, 47, 48]. Because the valence and sea quark actions are different, such calculations are inherently partially quenched and are not unitary. This type of calculation is sometimes referred to as the mixed action scheme. Unlike conventional partially quenched calculations, which become unitary when the valence quark mass is tuned to the sea quark mass, unitarity cannot be restored by tuning the valence quark mass. The next best option is to tune the valence quark mass in such a way that the resulting pions have the same mass as those made of the sea Kogut-Susskind fermions. In this case unitarity should be restored in the continuum limit, where the $n_f = 2 + 1$ staggered action has an $SU(12)_L \otimes SU(12)_R \otimes U(1)_V$ chiral symmetry due to the four-fold taste degeneracy of each flavor, and each π , K or η has 15 degenerate additional partners. At finite lattice spacing this symmetry is broken and the taste multiplets are no longer degenerate, but have splittings that are $\mathcal{O}(\alpha^2 t^2)$ [20, 21, 49, 50, 51]. The domain wall fermion mass is tuned to give valence pions (kaons) that match the Goldstone Kogut-Susskind pion (kaon)⁴. This choice gives pions that are as light as possible, resulting in better convergence of the χ -PT extrapolation of the lattice results to the physical quark mass point. This tuning was used by the LHPC collaboration [44, 45, 46, 47, 52, 53].

2.1.2 *Anisotropic Clover Wilson Fermions*

Recently anisotropic lattices have proven useful for spectroscopy projects, and as the calculations needed for studying multi-hadron systems rely on spectroscopy, NPLQCD has recently adopted clover-improved Wilson fermion actions. In particular, the $n_f = 2 + 1$ flavor anisotropic Clover Wilson action [54, 55] with stout-link smearing [56] of the spatial gauge fields in the fermion action with a smearing weight of $\rho = 0.14$ has been used. The gauge fields entering the fermion action are not smeared in the time direction, thus preserving the ultra-locality of the action in the time direction. Further, a tree-level tadpole-improved Symanzik gauge action with no 1×2 rectangle in the time direction is used. Anisotropy allows for a better extraction of the excited states as well as additional confidence that plateaus in the effective mass plots formed from the correlation functions (discussed in Section 2.2) have been observed, significantly reducing the systematic errors in observables due to fitting. The gauge field generation is done by the Hadron Spectrum Collaboration (HSC), and these gauge field configurations have been used for excited hadron spectrum calculations by HSC [57, 58, 59, 60].

⁴This is the only Goldstone boson that becomes massless in the chiral limit at finite lattice spacing.

2.2 Euclidean Space Correlation Functions

Most Euclidean space correlation functions computed in LQCD calculations (suitably Fourier transformed) are the sums of exponential functions. The arguments of the exponentials are the product of Euclidean time with the eigenvalues of the Hamiltonian associated with eigenstates in the finite-volume that couple to the hadronic sources and sinks. For a lattice that has infinite extent in the time-direction, the correlation function at large times becomes a single exponential dictated by the ground state energy and the overlap of the source and sink with the ground state. As an example, consider the pion two-point function, $C_{\pi^+}(t)$, generated by a source (and sink) of the form $\pi^+(\mathbf{x}, t) = \bar{u}(\mathbf{x}, t)\gamma_5 d(\mathbf{x}, t)$,

$$C_{\pi^+}(t) = \sum_{\mathbf{x}} \langle 0 | \pi^-(\mathbf{x}, t) \pi^+(\mathbf{0}, 0) | 0 \rangle \quad , \quad (14)$$

where the sum over all lattice sites at each time-slice, t , projects onto the $\mathbf{p} = \mathbf{0}$ spatial momentum states. The source $\pi^+(\mathbf{x}, t)$ not only produces single pion states, but also all states with the quantum numbers of the pion. More generally, the source and sink are smeared over lattice sites in the vicinity of (\mathbf{x}, t) to increase the overlap onto the ground state and lowest-lying excited states. Translating the sink operator in time via $\pi^+(\mathbf{x}, t) = e^{\hat{H}t} \pi^+(\mathbf{x}, 0) e^{-\hat{H}t}$, and inserting a complete set of states, gives ⁵

$$C_{\pi^+}(t) = \sum_n \frac{e^{-E_n t}}{2E_n} \sum_{\mathbf{x}} \langle 0 | \pi^-(\mathbf{x}, 0) | n \rangle \langle n | \pi^+(\mathbf{0}, 0) | 0 \rangle \rightarrow A_0 \frac{e^{-m_\pi t}}{2m_\pi} \quad . \quad (15)$$

At finite lattice spacing, the correlation functions for Wilson fermions remain sums of exponential functions, but for particular choices of parameters used in the domain-wall discretization, the correlation functions exhibit additional sinusoidally modulated exponential behavior at short-times with a period set by the lattice spacing [61].

It is straightforward to show that the lowest energy eigenvalue extracted from the correlation function in Eqs. (14) and (15) corresponds to the mass of the π^+ (and, more generally, the mass of the lightest hadronic state that couples to the source and sink) in the finite volume. The masses of stable single particle states can be extracted from a Lattice QCD calculation with high accuracy as long as the lattice spatial extent is large compared to the pion Compton-wavelength ⁶.

Once a correlation function is calculated, a common objective is to extract the argument of the exponential function that persists at large times. One way to do this is to simply fit the function over a finite number of time-slices to a single exponential function. A second method, that is somewhat more useful in visually assessing the quality of the calculation, is to form the effective mass (EM) function, e.g

$$M_{\text{eff.}}(t; t_J) = \frac{1}{t_J} \log \left(\frac{C_{\pi^+}(t)}{C_{\pi^+}(t + t_J)} \right) \rightarrow m_\pi \quad , \quad (16)$$

where both t and $M_{\text{eff.}}(t; t_J)$ are in lattice units. At large times, $M_{\text{eff.}}(t; t_J)$ becomes a constant equal to the mass of the lightest state contributing to the correlation function ⁷. The anti-periodic boundary-conditions in the time-direction, imposed on the quark-fields in order to recover the correct fermionic partition function, result in the single meson correlation functions being periodic in the time direction

⁵We assume the absence of external electroweak fields that may exert forces on hadrons in the lattice volume.

⁶Finite-volume effects are exponentially suppressed [62] by factors of $e^{-m_\pi L}$.

⁷This is obviously the most simplistic approach to this problem. One well-known method to extract the ground state and excited state energies is that of Lüscher and Wolff [63, 65] in which the correlation functions resulting from different sources and sinks are calculated. The resulting matrix of correlation functions is diagonalized, and the EM function for each resulting eigenvalue can be used to extract the spectrum.

and symmetric about the mid-point in the time direction. They are the sum of cosh-functions, and for such correlation functions it is useful to construct the EM using

$$M_{\text{eff.}}(t; t_J) = \frac{1}{t_J} \cosh^{-1} \left(\frac{C_{\pi^+}(t + t_J) + C_{\pi^+}(t - t_J)}{2 C_{\pi^+}(t)} \right) \rightarrow m_{\pi} \quad , \quad (17)$$

which becomes a constant value for a single exponential or a single hyperbolic-cosine (near the mid-point of the time-direction of the lattice).

2.3 Statistical Analysis Methods

Since Monte-Carlo integration is used to compute the relevant correlation functions, the statistical uncertainty must be carefully determined. The main observables extracted from the calculations presented in this review are energy eigenvalues and their differences, which contain information about phase shifts, scattering lengths and the three body interaction. The extraction of energy eigenvalues is done by fitting the relevant correlation functions to a sum of exponentials (or hyperbolic cosine functions). The optimal values for the energy are extracted from correlated χ^2 -minimization fits that take into account the time correlations in the lattice calculations. In particular, the relevant parameters, such as the energies and the amplitude of each state that contributes to the correlation function, are determined as those that minimize

$$\chi^2(A) = \sum_{ij} [\bar{G}(t_i) - F(t_i, A)] C_{ij}^{-1} [\bar{G}(t_j) - F(t_j, A)] \quad , \quad (18)$$

where $\bar{G}(t)$ are the lattice two point correlation functions, $F(t, A)$ are the fitting functions used, A denotes the set of fitting parameters over which $\chi^2(A)$ is minimized, and C_{ij} is the covariance matrix. The lattice two point correlation functions are determined as averages over N Monte-Carlo samples of the correlation function, $G_k(t)$:

$$\bar{G}(t) = \frac{1}{N} \sum_{k=1}^N G_k(t) \quad , \quad (19)$$

and

$$C_{ij} = \frac{1}{N(N-1)} \sum_{k=1}^N [G_k(t_i) - \bar{G}(t_i)] [G_k(t_j) - \bar{G}(t_j)] \quad . \quad (20)$$

The (standard) errors on the fitted parameters are determined by the boundaries of the error ellipsoid ⁸.

In computing scattering parameters, the procedure for determining the statistical uncertainties is somewhat more involved due to the highly non-linear relation between the scattering amplitude and the energy levels of the two-hadron system. First, one is interested in the energy differences between the energy levels of the two-hadron system and the sum of the masses of the two free hadrons (similarly for the case of three or more hadrons). These energy differences can be determined in two ways. The simplest is where ratios of correlators are constructed in such a way so that they are a sum over exponentials parametrized by the desired energy splittings. In this case Jackknife is used to determine the covariance matrix and then a correlated χ^2 -fit is performed. For a single elimination Jackknife, the covariance matrix of a ratio of correlation functions is

$$C_{ij} = \frac{N-1}{N} \sum_{k=1}^N [R_k(t_i) - \bar{R}(t_i)] [R_k(t_j) - \bar{R}(t_j)] \quad (21)$$

⁸For a pedagogical presentation of fitting see the TASI lectures by D. Toussaint [64].

where R_k is the desired ratio computed with the k th sample omitted from the full ensemble and \bar{R} is the ratio computed on the full ensemble.

Fitting correlation functions to the sum of p exponential functions to extract the ground state energy requires fitting ranges that start at time separations from the source that are large enough so that the $p+1^{\text{th}}$ and higher excited states have negligible contributions. The determination of the minimum time separation that can be included in the fit is sometimes subjective. Hence a systematic uncertainty due to the choice of the minimum time separation in the fit is included. This uncertainty is determined by observing the variation of the extracted results as a function of the choice of fitting interval. The final uncertainties include both systematic and statistical uncertainties combined in quadrature.

2.4 *Developments in Fitting Methodology*

Fitting correlation functions to a sum of exponentials is a notoriously hard problem. However, the fitting is greatly simplified and more robust if only the lowest energy eigenvalue is to be extracted. With this restriction, only a limited amount of information about the spectral properties of the theory can be extracted from the computed correlation functions and, in addition, control of the systematic uncertainties of the extracted ground state energy eigenvalue is somewhat limited. Because the statistical uncertainties in baryon correlation functions grow exponentially with Euclidean time at large times, extracting the lowest energy eigenvalue at large time separations (in order to reduce the systematic uncertainty due to the contamination from excited states) typically results in large statistical uncertainties. In other words one can trade statistical uncertainty growth for systematic uncertainty reduction. There are two approaches in resolving this problem. One is to develop better sampling methods to reduce statistical uncertainties in the correlation functions. Such techniques have been developed in simple lattice field theories such as spin systems (cluster algorithms). However, of the general correlation functions computed in Lattice QCD only one approach seems viable at this point. This is to extract as much information from the correlation functions at short time separations where the statistical noise does not overwhelm the signal. In this region, multiple exponentials contribute to the correlation functions, and although the general multi-exponential fit problem is difficult and not well behaved, correlation functions can be designed so that such fits are facilitated. Variational analysis on symmetric positive definite matrices of correlation functions has been successfully used in the Lattice QCD community to extract the energy eigenvalues contributing to the correlation functions (the Lüscher-Wolff method). These methods were originally introduced in Refs. [63, 65], and have been subsequently developed [57, 66, 67, 68].

2.4.1 *The Prony Method*

A simple and widely used method of estimating the mass of the ground state energy contributing to a correlation function is the EM, as given in Eq. (16). It is conventional to define the EM from the logarithm of the ratio of the correlation function on adjacent time-slices. It is also possible⁹ to form a more general EM from time-slices separated by $t_J > 1$. For exponentially decreasing signals with time-independent noise, this will naturally reduce the statistical uncertainty in the EM and improve the extraction of energy eigenvalues as it increases the “lever-arm” of the exponential. In such a case, the uncertainty in $M_{\text{eff}}(t; t_J)$ in Eq. (16) will decrease as $1/t_J$. Simple correlation functions involving pions have time-independent uncertainties, but this is not the case for baryonic correlation functions, whose relative uncertainties grow exponentially with time at large times. Improvements to baryon EMs, and ultimately the extraction of baryon masses and the energy eigenvalues in the volume, that result from $t_J > 1$ have been explored [74]. In fitting an energy to an EM (and other generalizations), either the Bootstrap or Jackknife procedures are used to generate the covariance matrix associated with the

⁹This was suggested by K. Juge in a talk at Lattice 2008, see Ref. [69], but may have been used earlier.

time-slices in the range of the fit. This covariance matrix is then used to form the χ^2/dof and extract the best estimate of the mass as well as its uncertainty by using methods described in Sec. 2.3.

Based on the findings of NMR spectroscopists, the EM method has been generalized to two or more exponential functions [70]¹⁰, and is found to compare favorably [73] to the variational approach. A detailed study of this approach in the analysis of correlation functions with small statistical uncertainties was performed in Ref. [74]. The method was found to be quite stable and to provide a simple and reliable method of determining the lowest energy eigenvalue. This is in contrast to an analysis of low-statistics correlation functions for which the method is quite unstable.

2.4.2 The Matrix-Prony Method

In Lattice QCD, it is simple and “cost” effective to construct a set of correlation functions with the same source (creation operator) interpolating field and several interpolating fields at the sink (annihilation operator). Multiple sinks and one source have been used for achieving the high statistics required to study multi-hadron systems. In this case, it is straightforward to generalize Prony’s method to include all correlation functions with the same source, and we call this the matrix-Prony method. This method leads to a further reduction in the uncertainty of the extraction of the energy eigenvalues. A similar approach has been briefly discussed in Ref. [75]. While the matrix-Prony method provides a computational simplification in the analysis of multiple correlation functions, and provides a tool with which to extract multiple energy eigenvalues and eigenstates from a single source, it should not be considered to be more reliable than the Lüscher-Wolff method [63, 65].

Assume there are N correlation functions¹¹ from which the lowest lying energy eigenvalues are desired. If these correlation functions are a sum of exponentials they satisfy the following recursion relation,

$$My(\tau + t_J) - Vy(\tau) = 0 \quad , \quad (22)$$

where M and V are $N \times N$ matrices and $y(t)$ is a column vector of N components corresponding to the N correlation functions. Eq. (22) implies that the correlation functions are

$$y(t) = \sum_{n=1}^N C_n q_n \lambda_n^t \quad , \quad (23)$$

where q_n and $\lambda_n = \exp(m_n t_J)$ are the eigenvectors and eigenvalues of the following generalized eigenvalue problem

$$Mq = \lambda Vq \quad . \quad (24)$$

Given the N sets of correlation functions, the energy eigenvalues can be found by determining the matrices M and V that are needed in order for the signal to satisfy Eq. (22). Solving Eq. (24) leads to the eigenvalues $\lambda_n = \exp(m_n t_J)$ and the eigenvectors q_n that are needed to reconstruct the amplitudes with which each exponential enters the correlation functions. A simple solution can be constructed as follows. First note that

$$M \sum_{\tau=t}^{t+t_W} y(\tau + t_J) y(\tau)^T - V \sum_{\tau=t}^{t+t_W} y(\tau) y(\tau)^T = 0 \quad . \quad (25)$$

Clearly, a solution for M and V is

$$M = \left[\sum_{\tau=t}^{t+t_W} y(\tau + t_J) y(\tau)^T \right]^{-1} \quad , \quad V = \left[\sum_{\tau=t}^{t+t_W} y(\tau) y(\tau)^T \right]^{-1} \quad , \quad (26)$$

¹⁰ The method is more generally referred to as Prony’s method [71] after Gaspard Riche de Prony who first constructed it in 1795 [72]. These techniques and other related methods are known as linear prediction theory in the signal analysis community.

¹¹We have applied the method for $N = 2$ and 3.

where these inverses exist provided that the range, t_W , is large enough to make the matrices in the brackets full rank ($t_W \geq N - 1$). Once the eigenvalues, λ_n and eigenvectors q_n are determined, the amplitudes, C_n , can be reconstructed using t as a normalization point. The shift parameter t_J can be used to improve stability and understand systematic effects. The above solution is equivalent to determining M and V by requiring that

$$\Psi^2 = \sum_{\tau=t}^{t+t_W} [My(\tau + t_J) - Vy(\tau)]^T [My(\tau + t_J) - Vy(\tau)] \quad (27)$$

is minimized.

To go beyond extracting N states, a second order recursion relation can be constructed and solved. The minimization condition of Eq. (27), augmented to contain the second order terms in the recursion, can be used to determine the unknown matrices. The resulting eigenvalue problem is a second order nonlinear generalized eigenvalue problem which is straightforward to solve. However, tests show that this approach is unstable and hence such analyses are restricted to extract, at most, N energies from N correlation functions.

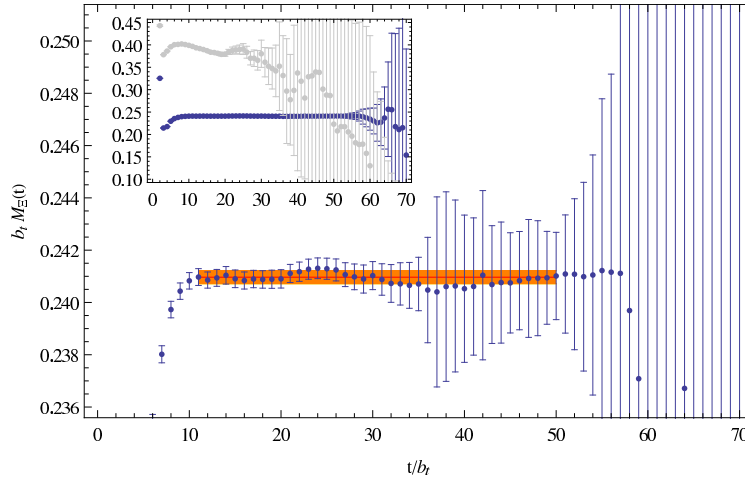


Figure 2: The generalized EMP for the mass of the Ξ using a Matrix-Prony analysis [74]. The correlation function was calculated on the $20^3 \times 128$ anisotropic clover gauge field configurations with $m_\pi \sim 390$ MeV. The inner (darker) region corresponds to the statistical uncertainty, while the outer (lighter) region corresponds to the statistical and fitting systematic uncertainties combined in quadrature. The inset shows the energies of both states extracted with the matrix-Prony method.

To demonstrate how this method works, results from the Ξ baryon correlation function calculated on the $20^3 \times 128$ anisotropic clover gauge field configurations with $m_\pi \sim 390$ MeV are presented. Figure 2 shows the generalized effective mass plot (EMP) for the Ξ mass as a function of time determined with a $N = 2$ matrix-Prony extraction, using both the smeared-smeared (SS) and smeared-point (SP) correlation functions. The inset shows the second extracted state in addition to the ground state. The extracted value of the Ξ mass, determined by fitting in the time interval $t = 11$ to $t = 50$, is

$$M_\Xi = 0.24097 \pm 0.00025 \pm 0.00003 \quad , \quad \chi^2/\text{dof} = 0.81 \quad . \quad (28)$$

The energy of the dominant state in Figure 2 plateaus around time-slice $t = 10$, and is well-defined over a large interval.

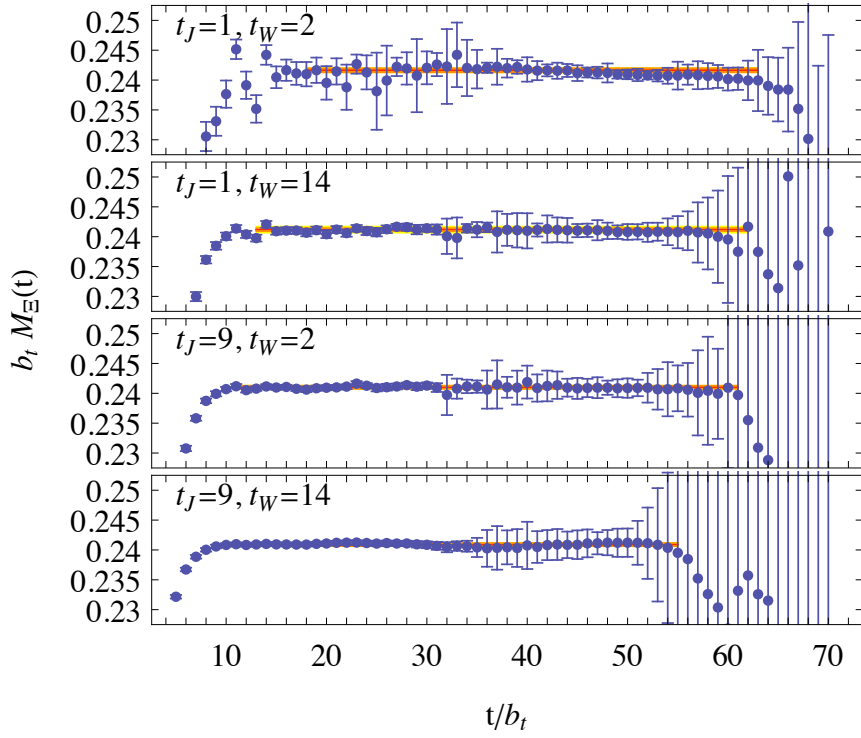


Figure 3: The generalized EMP for the mass of the Ξ using a Matrix-Prony analysis for a variety of values for t_J and t_W .

The matrix-Prony method is currently our preferred approach in analyzing correlation functions. Detailed tests of this method were presented in Ref. [74], which yield ground state energies that are in agreement with those from the other methods. The procedure for fitting parameters and determining their statistical uncertainty has been described in Section 2.3. Systematic uncertainties can be calculated by performing fits over rolling windows of time-slices within the quoted overall range and considering the standard deviation of the central values of those fits. This is combined in quadrature with a further systematic uncertainty that is generated by sampling a large range of possible values of t_J and t_W and taking the standard deviation of the central values of the resulting fits. The generalized EMP for the Ξ extracted with the matrix-Prony method for a variety of values of t_W and t_J can be seen in Figure 3. One further aspect of this method, that is perhaps the most appealing, is that the correlation functions corresponding to the eigenstates of the matrix-Prony matrix with lowest energy eigenvalue are dominated by the ground-state in the lattice volume, and hence have the longest plateau in the EMP. The EM corresponding to the eigenstates of the octet-baryons calculated on the $20^3 \times 128$ anisotropic clover gauge field configurations with $m_\pi \sim 390$ MeV are shown in Figure 4 (compared with Figure 2 and Figure 3).

2.5 Hadronic Interactions, the Maiani-Testa Theorem and Lüscher's Method

Extracting hadronic interactions from Lattice QCD calculations is far more complicated than the determination of the spectrum of stable particles. This is encapsulated in the Maiani-Testa theorem [76], which states that S-matrix elements cannot be extracted from infinite-volume Euclidean-space Green functions except at kinematic thresholds. This is clearly problematic from the nuclear physics perspective, as a main motivation for pursuing Lattice QCD is to be able to compute nuclear reactions involving multiple nucleons. Of course, it is clear from the statement of this theorem how it can be

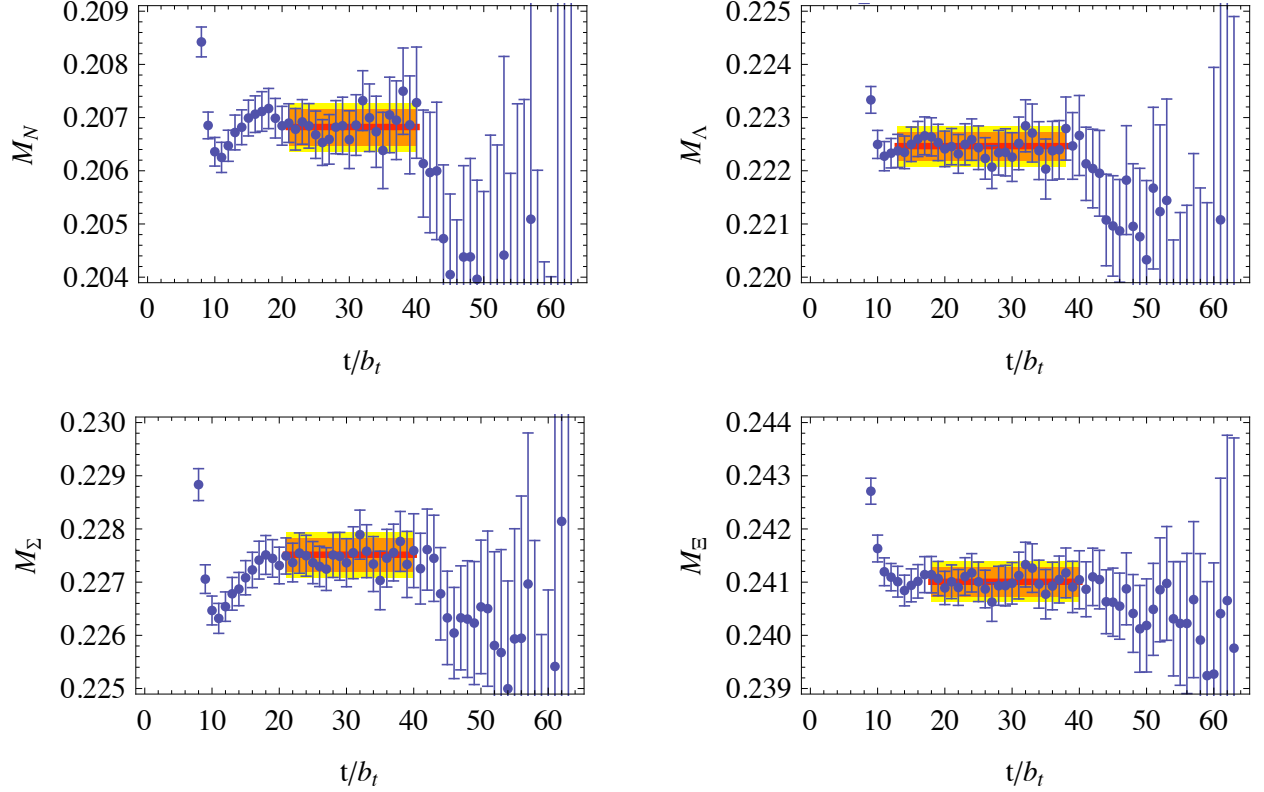


Figure 4: The EMPs for the masses of the octet-baryons from the eigenstates of a 2×2 matrix-Prony analysis of the SS and SP correlation functions [74] calculated on the $20^3 \times 128$ anisotropic clover gauge field configurations with $m_\pi \sim 390$ MeV.

evaded, Euclidean-space correlation functions are calculated at finite volume to extract S-matrix elements, the formulation of which was known for decades in the context of non-relativistic quantum mechanics [77] and extended to quantum field theory by Lüscher [78, 79]. The energy of two particles in a finite volume depends in a calculable way upon their elastic scattering amplitude and their masses for energies below the inelastic threshold. As a concrete example consider $\pi^+\pi^+$ scattering. A $\pi^+\pi^+$ correlation function in the A_1 representation of the cubic group [80] (that projects onto the continuum s-wave state amongst others) is

$$C_{\pi^+\pi^+}(p, t) = \sum_{|\mathbf{p}|=p} \sum_{\mathbf{x}, \mathbf{y}} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \langle \pi^-(t, \mathbf{x}) \pi^-(t, \mathbf{y}) \pi^+(0, \mathbf{0}) \pi^+(0, \mathbf{0}) \rangle . \quad (29)$$

In relatively large lattice volumes, the energy difference between the interacting and non-interacting two-meson states is a small fraction of the total energy, which is dominated by the masses of the mesons. This energy difference can be extracted from the ratio of correlation functions, $G_{\pi^+\pi^+}(p, t)$, where

$$G_{\pi^+\pi^+}(p, t) \equiv \frac{C_{\pi^+\pi^+}(p, t)}{C_{\pi^+}(t)C_{\pi^+}(t)} \rightarrow \mathcal{B}_0 e^{-\Delta E_0 t} , \quad (30)$$

and where the arrow denotes the large-time behavior of $G_{\pi^+\pi^+}$. For calculations performed with $p = 0$, the energy eigenvalue, E_n , and its deviation from the sum of the rest masses of the particle, ΔE_n , are related to a momentum magnitude p_n by

$$\Delta E_n \equiv E_n - 2m_\pi = 2\sqrt{p_n^2 + m_\pi^2} - 2m_\pi . \quad (31)$$

To obtain $k \cot \delta(k)$, where $\delta(k)$ is the phase shift, the square of p_n is extracted from the energy shift and inserted into [77, 78, 79, 81]

$$k \cot \delta(k) = \frac{1}{\pi L} \mathbf{S} \left(\left(\frac{kL}{2\pi} \right)^2 \right) , \quad \mathbf{S}(x) \equiv \sum_{|\mathbf{j}| < \Lambda} \frac{1}{|\mathbf{j}|^2 - x} - 4\pi\Lambda , \quad (32)$$

where $k = p_n$, and which is only valid below the inelastic threshold. The regulated three-dimensional sum [82] extends over all triplets of integers \mathbf{j} such that $|\mathbf{j}| < \Lambda$ and the limit $\Lambda \rightarrow \infty$ is implicit. Therefore, by calculating the energy-shift, ΔE_n , of the two particles in the finite lattice volume, the scattering phase-shift is determined at ΔE_n . In the absence of interactions between the particles the energy eigenstates in the finite volume occur at momenta $\mathbf{p} = 2\pi\mathbf{j}/L$. It is important to re-emphasize that the relation in Eq. (32) is valid relativistically [78, 79]. Perhaps most important for nuclear physics is that this expression is valid for large and even infinite scattering lengths [82]. The only restriction is that the lattice volume be much larger than the range of the interaction between the hadrons, which for two nucleons, is set by the mass of the pion.

For the scattering of two nucleons, the scattering length is known to be unnaturally large at the physical pion mass, and therefore, the relation in Eq. (32) will have to be used to extract the scattering parameters. For systems that are not finely-tuned, such as the $\pi^+\pi^+$ system, an expansion in the volume can be used. In the large volume limit ($L \gg |a|$) the energy of the two lowest-lying continuum states in the A_1 representation of the cubic group [80] are [78, 79]

$$\begin{aligned} \Delta E_0 &= +\frac{4\pi a}{ML^3} \left[1 - c_1 \frac{a}{L} + c_2 \left(\frac{a}{L} \right)^2 + \dots \right] + \mathcal{O}(L^{-6}) \\ \Delta E_1 &= \frac{4\pi^2}{ML^2} - \frac{12 \tan \delta_0}{ML^2} [1 + c'_1 \tan \delta_0 + c'_2 \tan^2 \delta_0 + \dots] + \mathcal{O}(L^{-6}) , \end{aligned} \quad (33)$$

where δ_0 is the s-wave phase-shift evaluated at $p = 2\pi/L$. The coefficients, which result from sums over the allowed momenta [78, 79] in the finite cubic volume, are $c_1 = -2.837297$, $c_2 = +6.375183$, $c'_1 = -0.061367$, and $c'_2 = -0.354156$ ¹². In addition, for $a > 0$ with an attractive interaction a bound state exists with energy [82] (in the large volume limit)

$$\Delta E_{-1} = -\frac{\gamma^2}{M} \left[1 + \frac{12}{\gamma L} \frac{1}{1 - 2\gamma(p \cot \delta)'} e^{-\gamma L} + \dots \right] , \quad (34)$$

where $(p \cot \delta)' = \frac{d}{dp^2} p \cot \delta$ evaluated at $p^2 = -\gamma^2$. The quantity γ is the solution of

$$\gamma + p \cot \delta|_{p^2 = -\gamma^2} = 0 , \quad (35)$$

which yields the bound-state binding energy in the infinite-volume limit. As expected, the finite volume corrections are exponentially suppressed by the binding momentum¹³. This is consistent with the corrections to a single particle state where the lightest hadronic excitation is the zero-momentum two-particle continuum state, as opposed to a state containing an additional pion for, say, the finite volume corrections to the single nucleon mass.

In the limit where $L \ll |(p \cot \delta)^{-1}|$, which is a useful limit to consider when systems have unnaturally-large scattering lengths, the solution of Eq. (32) gives the energy of the lowest-lying states:

$$\Delta \tilde{E}_0 = \frac{4\pi^2}{ML^2} [d_1 + d_2 L p \cot \delta_0 + \dots] , \quad \Delta \tilde{E}_1 = \frac{4\pi^2}{ML^2} [d'_1 + d'_2 L p \cot \delta_0 + \dots] , \quad (36)$$

¹²We use the nuclear physics sign convention for the scattering length.

¹³The finite volume dependence of bound states has been explored numerically in Ref. [83].

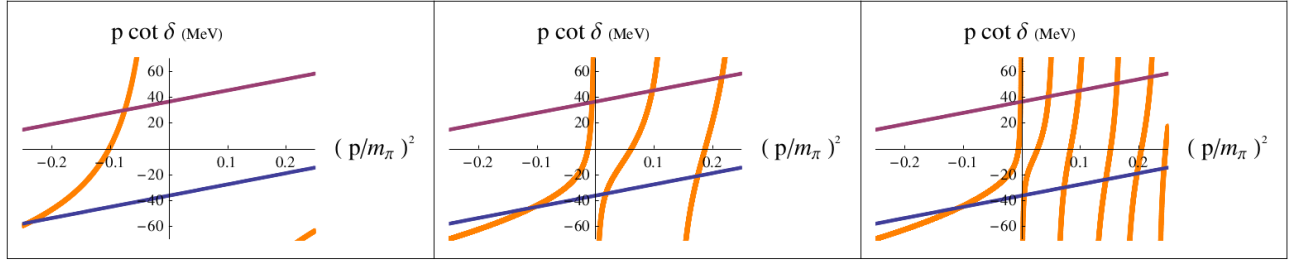


Figure 5: The functions $\mathbf{S}(x)$ (curved orange lines) and $p \cot \delta$ (straight red and blue lines) versus $(p/m_\pi)^2$ at the physical pion mass. The lower (blue) straight line corresponds to using the experimentally determined 3S_1 -channel nucleon-nucleon scattering length and effective range, while the upper (red) straight line corresponds to using a scattering length of opposite sign but equal magnitude. The left, center and right panels corresponds to lattices with spatial extent of $L = 8.5$ fm, 24.5 fm and 36.8 fm, respectively. The intercepts of the curves corresponds to the energy eigenvalues in the finite volume.

where the coefficients are $d_1 = -0.095901$, $d_2 = +0.0253716$, $d'_1 = +0.472895$, $d'_2 = +0.0790234$ and where $p \cot \delta_0$ in the expression for $\Delta \tilde{E}_0$ is evaluated at an energy $\Delta E = \frac{4\pi^2}{ML^2} d_1$, while $p \cot \delta_0$ in the expression for $\Delta \tilde{E}_1$ is evaluated at an energy $\Delta E = \frac{4\pi^2}{ML^2} d'_1$. The values of the $d_i^{(l)}$ are determined by zeros of $\mathbf{S}(x)$, and the expressions for ΔE_i and $\Delta \tilde{E}_i$, excluding ΔE_{-1} , are valid for both positive and negative scattering lengths.

2.6 Bound-States Versus Scattering-States

It is important to understand what can be extracted from finite-volume calculations. One important question that arises is: if a negative energy-shifted state is calculated on the lattice at finite-volume, does it correspond to a bound state or to a scattering state? Clearly, calculations of the same correlation function in multiple volumes will allow for the exponential volume dependence of a bound state to be distinguished from the power-law volume dependence of a scattering state. However, one can make an educated guess about the nature of the state by the magnitude of the energy shift. Consider a simple system whose scattering amplitude is dominated at low-energies by the scattering length and effective range, as is the case for the scattering of two nucleons. The location of the states in the lattice volume are determined by the solution of Eq. (32). In Figure 5 we show the graphical solution to Eq. (32) for two systems, one with $a = +5.425$ fm and $r = 1.749$ fm (blue line) and the other with $a = -5.425$ fm and $r = 1.749$ fm (red line). One finds that states with $E < 0$ and $p \cot \delta < 0$ (which occur for $x = \left(\frac{pL}{2\pi}\right)^2 < d_1$) likely correspond to a bound-state, while states with $E < 0$ and $p \cot \delta > 0$ ($x > d_1$) likely correspond to continuum states. However, one can imagine scattering parameters in the momentum expansion of $p \cot \delta$ that modify these rules.

The location of the bound-state and the first continuum state for two nucleons in the 3S_1 channel (neglecting D-wave interactions and mixing) as a function of lattice volume are shown in Figure 6. In order for the bound-state energy to be very close to that of the deuteron binding energy, the lattice volumes must be very large. However, as shown in Section 6, a single calculation of the lowest energy in the lattice volume is not the best way to determine the deuteron binding energy. The deuteron binding energy will best be determined from the calculation of ground-state and continuum state energies in one or more lattice volumes.

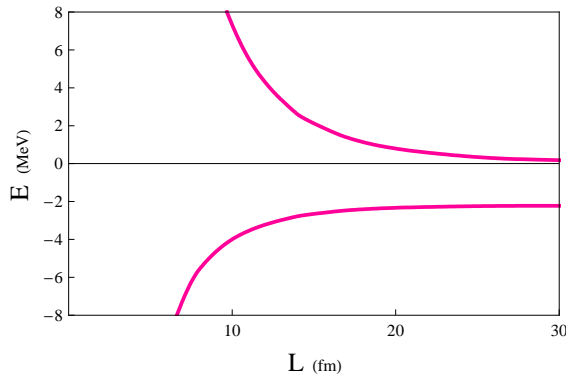


Figure 6: The energy of the bound-state and first continuum state of two nucleons in the 3S_1 channel (neglecting D-wave interactions and mixing) as a function of the spatial extent of the lattice (fm).

2.7 Scattering Parameters from Wavefunctions.

One remarkable feature of nuclear physics is that one can understand and compute (to reasonable accuracy) the properties and interactions of nuclei working with an energy-independent two-nucleon potential alone. Phenomenologically, one finds that the three-nucleon interaction, and, in the case of electroweak matrix elements, meson exchange currents, are required to improve agreement with experiment. But the fact remains that the two-nucleon potential is the dominant interaction in nuclei. There is a desire to construct such nucleon-nucleon potentials ¹⁴ directly from QCD, and hence from Lattice QCD. Nucleon-nucleon potentials may be defined from Lattice QCD calculations in the same way that phenomenological potentials are determined from experimental measurements of the elastic scattering cross-section. A large number of Lattice QCD calculations will be performed, producing values for the phase shift, along with an uncertainty, over a wide range of low-energies. Potentials can be defined that minimize the χ^2/dof in a global fit to the calculated phase-shifts. At present, there is no practical program underway to perform such an analysis due to limited computational power.

The utility of two particle wavefunctions and potentials in LQCD calculations was first addressed in a substantive way by Lüscher [79]. The methodology outlined by Lüscher has been used by the CP-PACS collaboration in early work that determined scattering parameters and phase shift of the $\pi^+\pi^+$ system from quenched calculations at relatively large pion masses with Wilson fermions [84, 85]. Consider an interpolating operator for $\pi^+\pi^+$ states of the form

$$\hat{\theta}(\mathbf{x}, \mathbf{y}; t) = \bar{u}(\mathbf{x}, t) \gamma_5 d(\mathbf{x}, t) \bar{u}(\mathbf{y}, t) \gamma_5 d(\mathbf{y}, t) \quad , \quad (37)$$

where the quark-field operators $q(x)$ may be smeared about the point x to enhance the overlap of the single- π^+ interpolating operator, $\bar{u}(\mathbf{x}, t) \gamma_5 d(\mathbf{x}, t)$, onto the single- π^+ state. A $\pi^+\pi^+$ correlation function

$$\begin{aligned} G(|\mathbf{x}|, t) &= \frac{1}{48 L^3} \sum_{\mathbf{R}, \mathbf{y}} \langle \hat{\theta}(\mathbf{R}[\mathbf{x}] + \mathbf{y}, \mathbf{y}; t) \hat{\theta}^\dagger(\mathbf{0}, \mathbf{0}; 0) \rangle \\ &\rightarrow Z_{\pi\pi}(0; k) Z_{\pi\pi}(|\mathbf{x}|; k) e^{-E_{\pi\pi}^{(0)} t} \psi_{\pi\pi}(|\mathbf{x}|; k) \quad , \end{aligned} \quad (38)$$

can be constructed, where \mathbf{R} represents an element of the cubic group. The magnitude of momentum, k , is defined through $E_{\pi\pi}^{(0)} = 2\sqrt{k^2 + m_\pi^2}$, as in Eq. (31). The summation over \mathbf{R} and \mathbf{y} projects onto the

¹⁴In this context, the word *potential* means an energy-independent potential.

A_1 representation of the cubic-group with zero total momentum. We have performed a separation¹⁵ into the product of a sink-dependent overlap factor, $Z_{\pi\pi}(|\mathbf{x}|; k)$, and a hadronic wavefunction, $\psi_{\pi\pi}(|\mathbf{x}|; k)$. The spatially-dependent overlap factor $Z_{\pi\pi}(|\mathbf{x}|; k)$ is introduced in order to stress the fact that the overlap (onto a given eigenstate in the lattice volume) of the composite sink-operator $\hat{\theta}(\mathbf{R}[\mathbf{x}] + \mathbf{y}, \mathbf{y}; t)$ is not the square of the overlap of the interpolating operator for the single π^+ when $|\mathbf{x} - \mathbf{y}| \lesssim R$ where R is a typical strong interaction length scale set by the mass of the pion (i.e. it is set by the range of the interaction between two π^+ 's.). The wavefunction given in Eq. (38), $\phi(|\mathbf{x}|; k) \sim Z_{\pi\pi}(|\mathbf{x}|; k) \psi_{\pi\pi}(|\mathbf{x}|; k)$ satisfies the Schrodinger equation [79]

$$(\nabla^2 + k^2) \phi(|\mathbf{x}|; k) = \int d^3\mathbf{y} U_k(\mathbf{x}, \mathbf{y}) \phi(|\mathbf{y}|; k) , \quad (39)$$

where $U_k(\mathbf{x}, \mathbf{y})$ is the Fourier transform of the modified Bethe-Salpeter kernel for the $\pi^+\pi^+$ interaction, which is generally nonlocal and energy-dependent [79, 84, 85]. An investigation of this construction under the assumption that $U_k(\mathbf{x}, \mathbf{y})$ is independent of energy can be found in Ref. [86]. In the limit where the separation between the two π^+ 's is large compared to the range of the interaction (the inverse pion mass), $|\mathbf{x}| \gg R$, the normalization factor tends to constant value that is the product of the single- π^+ overlap factor, $Z_{\pi\pi}(|\mathbf{x}|; k) \rightarrow Z_\pi(k)^2$, and the non-local, energy-dependent kernel tends to zero, $U_k(\mathbf{x}, \mathbf{y}) \rightarrow 0$, leaving the hadronic wavefunction, $\psi_{\pi\pi}(|\mathbf{x}|; k)$, to satisfy the Helmholtz equation, $(\nabla^2 + k^2) \psi_{\pi\pi}(|\mathbf{x}|; k) = 0$. As the A_1 representation of the cubic-group projects onto angular momentum $l = 0, 4, 6, 8, \dots$, at low-momentum only s-wave scattering is significant and outside the range of the interaction the wavefunction becomes $\psi_{\pi\pi}(|\mathbf{x}|; k) = A_0 j_0(k|\mathbf{x}|) + B_0 n_l(k|\mathbf{x}|)$. The scattering phase shift is simply determined from $\tan \delta_0(k) = -B_0/A_0$. The CP-PACS collaboration has claimed that the uncertainty in the scattering length extracted from LQCD calculations of the asymptotic behavior of the $\pi^+\pi^+$ wavefunction is approximately two-thirds that of the extraction from the energy eigenvalue via the usual Lüscher-method [84, 85].

One can define an energy- and sink-dependent potential, defined at one energy (the energy of the two π^+ 's determined in the finite volume) through an uncontrolled modification to Eq. (39),

$$\frac{(\nabla^2 + k^2) \phi(|\mathbf{x}|; k)}{m_\pi \phi(|\mathbf{x}|; k)} = V_k(|\mathbf{x}|) , \quad (40)$$

but it is clear that, except in the case of infinitely massive hadrons [87], $V_k(|\mathbf{x}|)$ contains no more information than the phase shift at the energy determined with Lüscher's method¹⁶. One such potential for nucleon-nucleon scattering was calculated in quenched QCD in Ref [88] but, for the reasons detailed above, it cannot be used as an input in nuclear calculations and it cannot be meaningfully compared to phenomenological nucleon-nucleon potentials¹⁷. An investigation of the sink dependence

¹⁵Alternatively, we could have simply indicated that the wavefunction depends upon the sink by $\psi_{\pi\pi}(|\mathbf{x}|; k) \rightarrow \psi_{\pi\pi}^{(\theta)}(|\mathbf{x}|; k)$.

¹⁶The phase-shift is recovered by solving

$$(-\nabla^2 + m_\pi V_k(|\mathbf{x}|)) \phi(|\mathbf{x}|; k) = k^2 \phi(|\mathbf{x}|; k) , \quad (41)$$

at the calculated value of k^2 .

¹⁷The information content of the potentials derived from the analysis of hadron-hadron wavefunctions calculated with Lattice QCD is displayed by the following modifications to the method of Ref [88]. One could use wall-sinks for the two hadrons, $\bar{\mathcal{T}}^\dagger(0, t)$, by projecting each quark to have zero momentum. The interpolating operator has the same quantum numbers as that used in Ref [88] and the associated correlation function

$$\bar{G}(\mathbf{x}, t) = \langle 0 | \bar{\mathcal{T}}^\dagger(0, t) \bar{\mathcal{T}}(0, 0) | 0 \rangle , \quad (42)$$

is uniform over the spatial volume at each time-slice, and gives rise to a potential that is also uniform on each time-slice: $V_k(|\mathbf{x}|) = k^2/m$. This provides a clear demonstration of the fact that potentials extracted by such methods depend upon the choice of sink operator and are not unique predictions of QCD.

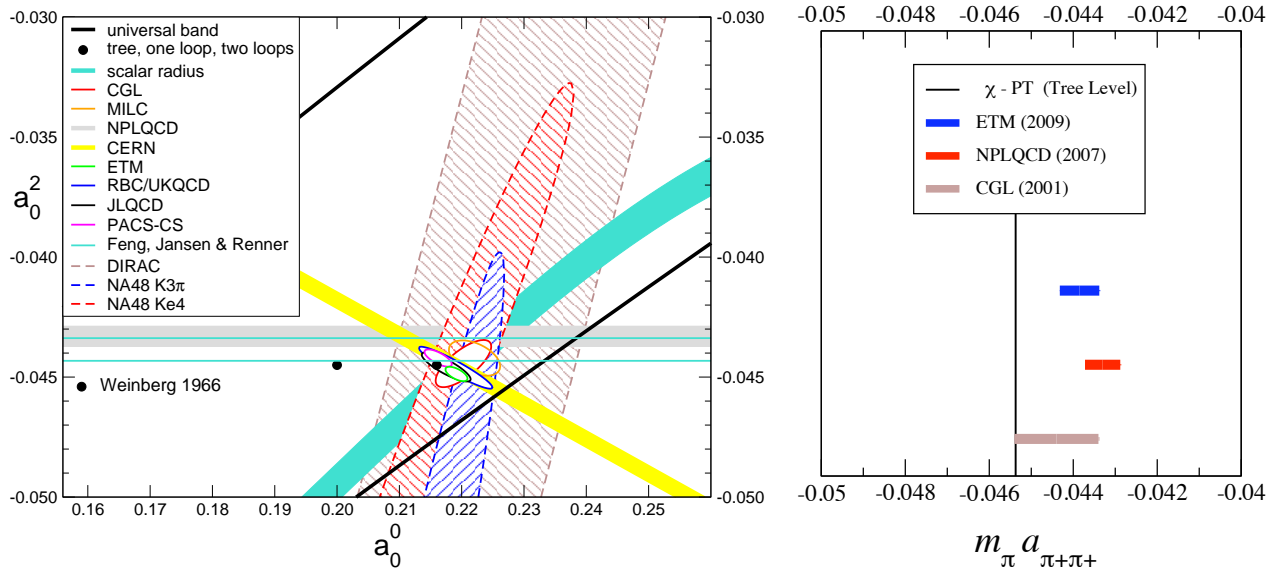


Figure 7: Present constraints on threshold s-wave $\pi\pi$ scattering. Noteworthy in the left panel [93] are the red hatched ellipse from the Roy equation analysis and the grey band from the direct Lattice QCD calculation of the $\pi^+\pi^+$ scattering length, as discussed in the text. The right panel shows the $\pi^+\pi^+$ scattering length results only (the ETM result is at the top, the NPLQCD result is in the middle and the CGL result is at the bottom).

of these potentials has been performed and presented in a set of lectures [89]. In this study, block spin transformations were applied to the quark fields used in the calculations and $\mathcal{O}(1)$ modifications to the potentials were found out to a distance of ~ 0.5 fm. Analogous energy- and sink-dependent potentials have been constructed for hyperon-nucleon scattering as well [90].

3 Two-Body Physics

3.1 Meson-Meson Interactions

The low-energy scattering of pions and kaons, the pseudo-Goldstone bosons of spontaneous chiral symmetry breaking, provides a perfect testing ground for Lattice QCD calculations of scattering parameters. There is little or no signal-to-noise problem in such calculations and therefore highly accurate Lattice QCD calculations can be performed with moderate resources. Moreover, the EFTs which describe the low-energy interactions of pions and kaons, including lattice-spacing and finite-volume effects, have been developed to non-trivial orders in the chiral expansion.

The $I = 2$ pion-pion ($\pi^+\pi^+$) scattering length serves as a benchmark calculation with an accuracy that can only be aspired to at present for other systems. Furthermore, due to the chiral symmetry of QCD, $\pi\pi$ scattering at low energies is the simplest and best-understood of the hadron-hadron scattering processes. The scattering lengths for $\pi\pi$ scattering in the s-wave are uniquely predicted at LO in χ -PT [91]:

$$m_\pi a_{\pi\pi}^{I=0} = 0.1588 ; \quad m_\pi a_{\pi\pi}^{I=2} = -0.04537 , \quad (43)$$

when m_π is set equal to the charged pion mass. While experiments do not directly provide stringent constraints on the scattering lengths, a determination of s-wave $\pi\pi$ scattering lengths using the Roy

equations has reached a remarkable level of precision [92, 93]:

$$m_\pi a_{\pi\pi}^{I=0} = 0.220 \pm 0.005 \quad ; \quad m_\pi a_{\pi\pi}^{I=2} = -0.0444 \pm 0.0010 \quad . \quad (44)$$

The Roy equations [94] use dispersion theory to relate scattering data at high energies to the scattering amplitude near threshold. At present, Lattice QCD can compute $\pi\pi$ scattering only in the $I = 2$ channel with precision as the $I = 0$ channel contains disconnected diagrams which require large computational resources. It is of great interest to compare the precise Roy equation predictions with Lattice QCD calculations. Figure 7 summarizes theoretical and experimental constraints on the s-wave $\pi\pi$ scattering lengths [93]. It is clearly a strong-interaction process where theory has somewhat out-paced the very challenging experimental measurements.

The only existing $n_f = 2 + 1$ Lattice QCD prediction of the $I = 2$ $\pi\pi$ scattering length involves a mixed-action Lattice QCD scheme of domain-wall valence quarks on a rooted staggered sea. Details of the lattice calculation can be found in Ref. [95]. The scattering length was computed at pion masses, $m_\pi \sim 290$ MeV, 350 MeV, 490 MeV and 590 MeV, and at a single lattice spacing, $b \sim 0.125$ fm and lattice size $L \sim 2.5$ fm [95]. The physical value of the scattering length was obtained using two-flavor mixed-action χ -PT which includes the effect of finite lattice-spacing artifacts to $\mathcal{O}(m_\pi^2 b^2)$ and $\mathcal{O}(b^4)$ [43]. The final result is:

$$m_\pi a_{\pi\pi}^{I=2} = -0.04330 \pm 0.00042 \quad , \quad (45)$$

where the statistical and systematic uncertainties have been combined in quadrature. Notice that this is a 1% calculation, but it does rely on the assumption that the rooting procedure used in the generation of the staggered gauge field configurations is valid, and also relies on mixed-action chiral perturbation theory at NLO to describe the lattice spacing artifacts. The agreement between this result and the Roy equation determination is a striking confirmation of the lattice methodology, and a powerful demonstration of the constraining power of chiral symmetry in the meson sector. However, lattice calculations at one or more smaller lattice spacings are required to verify and further refine this calculation. It is also desirable that the scattering amplitude be calculated with mixed-action chiral perturbation theory to one higher order in the lattice spacing in order to explore the convergence of this expansion.

It is of great importance to have other Lattice QCD determinations of the s-wave meson-meson scattering lengths which use different lattice discretizations. Very recently, the ETM collaboration has performed a $n_f = 2$ calculation of the $I = 2$ $\pi\pi$ scattering length at pion masses ranging from $m_\pi \sim 270$ MeV to 485 MeV, at two lattice spacings ($b \sim 0.086$ fm and $b \sim 0.067$ fm) and at two lattice sizes ($L \sim 2.1$ fm and $L \sim 2.7$ fm) [96]. The result extrapolated to the physical pion mass is:

$$m_\pi a_{\pi\pi}^{I=2} = -0.04385 \pm 0.00028 \pm 0.00038 \quad , \quad (46)$$

where the first uncertainty is statistical and the second is an estimate of systematic effects. The agreement among the Lattice QCD calculations and the Roy equation determination is striking. In Figure 8, the CP-PACS, NPLQCD and ETM Lattice QCD calculations of the $\pi^+\pi^+$ scattering length are shown with the LO χ -PT prediction subtracted. The shaded band corresponds to the NLO χ -PT fit to the lattice calculations.

It is interesting to consider the pion mass dependence of the meson-meson scattering lengths¹⁸ as compared to the current algebra predictions. In Figure 9 (left panel) one sees that the $I = 2$ $\pi\pi$

¹⁸ The K^+K^+ and π^+K^+ scattering lengths have also been computed by the NPLQCD collaboration. We refer the interested reader to Figure 9 and Figure 10, and to Ref. [97] for details. Exploratory calculations of πK scattering in both isospin channels have been recently performed using $n_f = 2 + 1$ improved Wilson quarks [98], and two quenched studies have also been performed [99, 100].

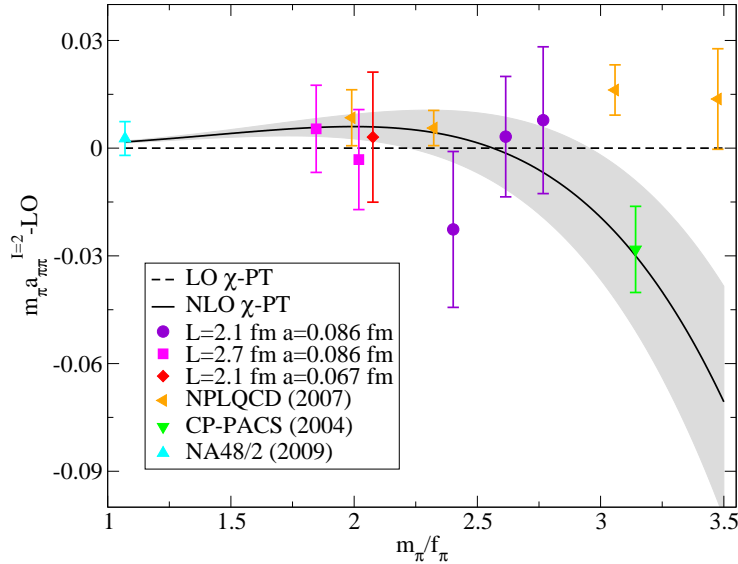


Figure 8: Lattice QCD calculations of the $\pi^+\pi^+$ scattering length with the LO χ -PT prediction removed [96]. The shaded band corresponds to the NLO χ -PT fit to the lattice calculations. The calculations with $L = 2.1$ fm and 2.7 fm were performed by the ETM collaboration [96].

scattering length is consistent with the current algebra result up to pion masses that are expected to be at the edge of the chiral regime in the two-flavor sector. While in the two flavor theory one expects fairly good convergence of the chiral expansion and, moreover, one expects that the effective expansion parameter is small in the channel with maximal isospin, the lattice calculations clearly imply a cancellation between chiral logs and counterterms (evaluated at a given scale). However, as one sees in Figure 9 (right panel), the same phenomenon occurs in K^+K^+ where the chiral expansion is governed by the strange quark mass and is therefore expected to be much more slowly converging. The π^+K^+ scattering length exhibits similar behavior when $\mu_{K\pi} a_{K^+\pi^+}$ is plotted against $\mu_{K\pi}/\sqrt{f_K f_\pi}$ as shown in Figure 10. This remarkable cancellation between chiral logs and counterterms for the meson-meson scattering lengths is quite mysterious.

One (very) naive interpretation of these results is that the contributions to these quantities from higher order terms in the chiral expansion are much smaller than one would naively anticipate, and this is not just a result of cancellation between terms. This leaves one with the task of understanding the origin of this suppression of the higher order terms. The totality of precision results may suggest that there is a dynamically induced length scale governing the size of contributions beyond tree-level that has yet to be understood.

3.2 Meson-Baryon Interactions

Pion-nucleon scattering has long been considered a paradigmatic process for the comparison of χ -PT and experiment. To this day, controversy surrounds determinations of the pion-nucleon coupling constant and the pion-nucleon sigma term. The K^-n interaction is important for the description of kaon condensation in the interior of neutron stars [101], and meson-baryon interactions are essential input in determining the final-state interactions of various decays that are interesting for standard model phenomenology (see Ref. [102] for an example). In determining baryon excited states on the lattice, it is clear that the energy levels that represent meson-baryon scattering on the finite-volume lattice must

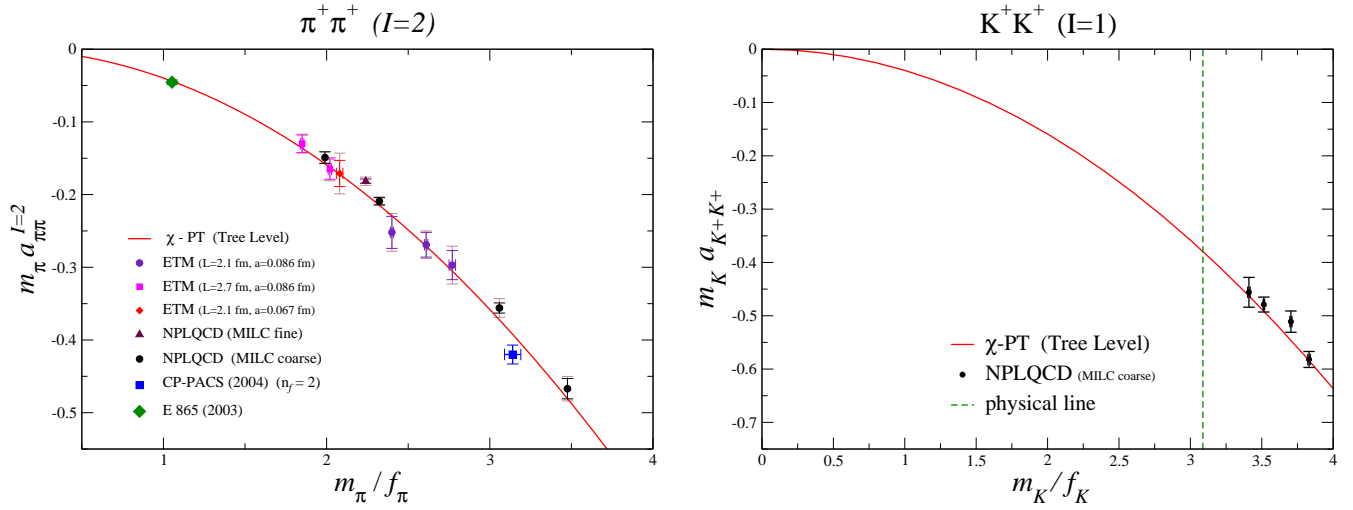


Figure 9: $m_\pi a_{\pi^+\pi^+}$ vs. m_π/f_π (left panel) and $m_K a_{K^+K^+}$ vs. m_K/f_K (right panel). The black (darker) circles and dark-brown triangles are the results of Lattice QCD calculations by the NPLQCD collaboration, the blue (darker) square (left panel) is from the CP-PACS collaboration, the purple (lighter) circles, red diamonds and magenta (lighter) squares (left panel) are from the ETM collaboration. The solid (red) lines are the current algebra predictions.

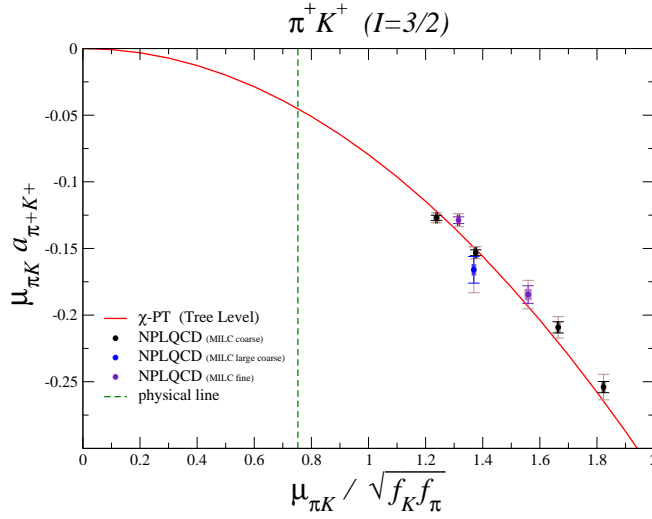


Figure 10: $\mu_{\pi K} a_{\pi^+K^+}$ vs. $\mu_{\pi K}/\sqrt{f_K f_\pi}$. The points are the results of Lattice QCD calculations by the NPLQCD collaboration and the solid (red) line is the current algebra prediction.

be resolved before progress can be made regarding the extraction of single-particle excitations.

While pion-nucleon scattering is the best-studied meson-baryon process, both theoretically and experimentally, its determination on the lattice is computationally prohibitive since it involves annihilation diagrams¹⁹. Combining the lowest-lying meson and baryon flavor octets, one can form five meson-baryon elastic scattering processes that do not involve annihilation diagrams: $\pi^+\Sigma^+$, $\pi^+\Xi^0$, K^+p ,

¹⁹In recent work, the s-wave πN phase-shift was extracted from the negative-parity single nucleon correlation function [74].

K^+n , and $\bar{K}^0\Xi^0$ ²⁰. Three of these processes involve kaons and therefore are, in principle, amenable to an $SU(3)$ HB χ -PT analysis [103] for extrapolation. The remaining two processes involve pions interacting with hyperons and therefore can be analyzed in conjunction with the kaon processes in $SU(3)$ HB χ -PT, or independently using $SU(2)$ HB χ -PT. An analysis of meson-baryon scattering using the mixed-action technology and resources was recently performed [104]. The scattering lengths of the five meson-baryon processes without annihilation diagrams have been calculated to $\mathcal{O}(m_{\pi,K}^3)$ in $SU(3)$ HB χ -PT [105, 106], and involve low-energy constants, the C 's and the h 's, and the loop functions, \mathcal{Y} 's, which are given in Ref. [104]. The system of processes is found to be over-constrained, and multiple fitting strategies are possible, as discussed in Ref. [104]. It is convenient to rewrite the χ -PT formulas as polynomial expansions. For instance, in the case of $\pi^+\Xi^0$, the NLO and next-to-next-to-leading-order (NNLO) polynomial expressions are

$$\begin{aligned}\Gamma_{\text{NLO}} &\equiv -\frac{4\pi f_\pi^2 a_{\pi^+\Xi^0}}{m_\pi} \left(1 + \frac{m_\pi}{M_\Xi}\right) = 1 - C_{01}m_\pi \\ \Gamma_{\text{NNLO}} &\equiv -\frac{4\pi f_\pi^2 a_{\pi^+\Xi^0}}{m_\pi} \left(1 + \frac{m_\pi}{M_\Xi}\right) + \frac{f_\pi^2}{m_\pi} \mathcal{Y}_{\pi^+\Xi^0}(\Lambda_\chi) = 1 - C_{01}m_\pi - 8h_1(\Lambda_\chi)m_\pi^2 \quad .\end{aligned}\quad (47)$$

The left-hand sides of these equations are given entirely in terms of lattice-determined quantities, while the right-hand side provides a convenient polynomial fitting function. Figure 11 shows the results of the Lattice QCD calculation, along with the fits. The shift of the value of Γ from NLO to NNLO is

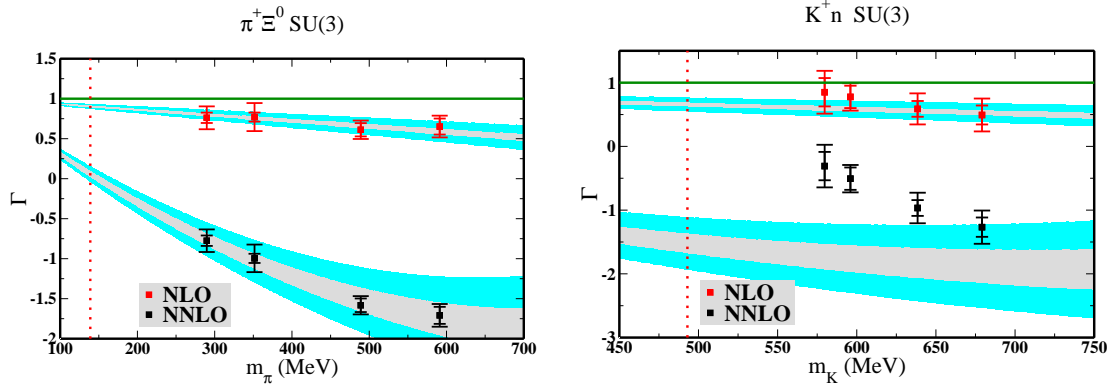


Figure 11: Γ_{NLO} and Γ_{NNLO} versus the meson masses for two of the meson-baryon processes in $SU(3)$ HB χ -PT. The line at $\Gamma = 1$ is the LO curve, and dotted line is the physical meson mass.

dependent on the renormalization scale μ , and therefore with the choice $\mu = \Lambda_\chi$ one would expect this shift to be perturbative if the expansion is converging. The large shifts in Γ from NLO to NNLO are indicative of large loop corrections. The low-energy constants (LECs) fit to the results of the lattice calculations are tabulated in Ref. [104]. While the NNLO LECs h_1 and h_{123} appear to be of natural size, the NLO LECs C_0 and C_{01} are unnaturally large. The extrapolated values of the five scattering lengths are given in Table 1. While the $\pi^+\Sigma^+$ and $\pi^+\Xi^0$ scattering lengths appear to be perturbative, the extrapolated kaon-baryon scattering lengths at NNLO deviate by at least 100% from the LO values. The seemingly inescapable conclusion is that the kaon-baryon scattering lengths are unstable against chiral corrections in the three-flavor chiral expansion, over the explored range of light-quark masses.

Given the poor convergence found in the three-flavor chiral expansion due to the large loop corrections, it is natural to consider the two-flavor theory with the strange quark integrated out. In this way,

²⁰ $\bar{K}^0\Sigma^+$ has the same quantum numbers as $\pi^+\Xi^0$.

Table 1: $SU(3)$ HB χ -PT extrapolated scattering lengths. The first uncertainty is statistical, and the second is the statistical and systematic uncertainty added in quadrature. “NLO (NNLO fit)” indicates that the C_1 and C_{01} from the NNLO fit to $\pi^+\Sigma^+$ and $\pi^+\Xi^0$ have been used.

Quantity	LO (fm)	NLO fit (fm)	NLO (NNLO fit) (fm)	NNLO (fm)
$a_{\pi\Sigma}$	-0.2294	-0.208(01)(03)	-0.117(06)(08)	-0.197(06)(08)
$a_{\pi\Xi}$	-0.1158	-0.105(01)(04)	0.004(05)(11)	-0.096(05)(12)
a_{Kp}	-0.3971	-0.311(18)(44)	0.292(35)(48)	-0.154(51)(63)
a_{Kn}	-0.1986	-0.143(10)(27)	0.531(28)(68)	0.128(42)(87)
$a_{K\Xi}$	-0.4406	-0.331(12)(31)	0.324(39)(54)	-0.127(57)(70)

$\pi\Sigma$ and $\pi\Xi$ may be analyzed in an expansion in m_π . To $\mathcal{O}(m_\pi^3)$ in the two-flavor chiral expansion, one has [107]

$$\begin{aligned}
a_{\pi^+\Sigma^+} &= \frac{1}{2\pi} \frac{m_\Sigma}{m_\pi + m_\Sigma} \left[-\frac{m_\pi}{f^2} + \frac{m_\pi^2}{f^2} C_{\pi^+\Sigma^+} + \frac{m_\pi^3}{f^2} h'_{\pi^+\Sigma^+} \right], & h'_{\pi^+\Sigma^+} &= \frac{4}{f^2} \ell_4^r + h_{\pi^+\Sigma^+}, \\
a_{\pi^+\Xi^0} &= \frac{1}{4\pi} \frac{m_\Xi}{m_\pi + m_\Xi} \left[-\frac{m_\pi}{f^2} + \frac{m_\pi^2}{f^2} C_{\pi^+\Xi^0} + \frac{m_\pi^3}{f^2} h'_{\pi^+\Xi^0} \right], & h'_{\pi^+\Xi^0} &= \frac{4}{f^2} \ell_4^r + h_{\pi^+\Xi^0},
\end{aligned} \quad (48)$$

where ℓ_4^r is the LEC which governs the pion mass dependence of f_π [92]. Note that the chiral logs have

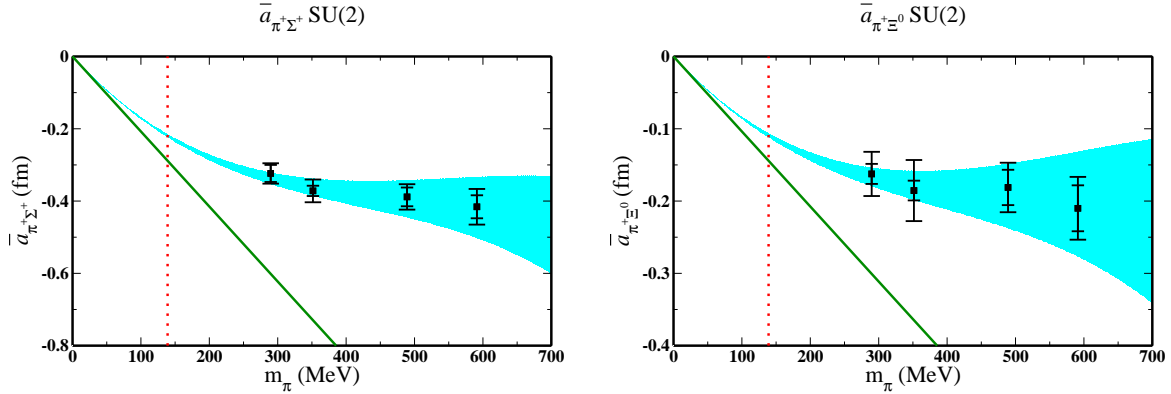


Figure 12: \bar{a} versus the pion mass for $\pi^+\Sigma^+$ and $\pi^+\Xi^0$. The diagonal line is the LO curve, and the dotted line is the physical pion mass. The innermost error bar is the statistical uncertainty and the outermost error bar is the statistical and systematic uncertainty added in quadrature. The filled bands correspond to the fits to the LECs in the $SU(2)$ case at NNLO.

canceled, and in this form, valid to order m_π^3 in the chiral expansion, the scattering lengths have a simple polynomial dependence on m_π [107]. Exploring the full 95% confidence interval error ellipse in the h - C plane yields pion-hyperon scattering lengths, extrapolated to the physical pion mass, of

$$a_{\pi^+\Sigma^+} = -0.197 \pm 0.017 \text{ fm}, \quad a_{\pi^+\Xi^0} = -0.096 \pm 0.017 \text{ fm}, \quad (49)$$

and the scattering length versus the pion mass is shown in Figure 12²¹.

²¹The bar denotes the scattering length rescaled by a kinematical factor [104].

The HB χ -PT analyses of meson-baryon scattering support a general observation about convergence in the three-flavor chiral expansion. As the pion masses considered in the lattice calculation are comparable to the physical kaon mass, the distinct convergence patterns of the two- and three-flavor chiral expansions are suggestive that the breakdown in the three-flavor case is not due to the relative largeness of the strange-quark mass as compared to the light quark masses, but rather due to some other enhancement in the coefficients of the loop contributions, possibly related to a scaling with powers of n_f , the number of flavors.

3.3 NN , YN and YY Interactions

Perhaps the most studied and best understood of the two-hadron processes are proton-proton and proton-neutron scattering. In the S-wave, only two combinations of spin and isospin are possible, a spin-triplet isosinglet np (3S_1) and a spin-singlet isotriplet pp (1S_0). At the physical pion mass, the scattering lengths in these channels are unnaturally large and the $^3S_1 - ^3D_1$ coupled-channel contains a shallow bound state, the deuteron, with a binding energy of ~ 2.22 MeV. These large scattering lengths and the shallow bound state are described, in EFT, by the coefficient of the momentum-independent four-nucleon operator having a non-trivial fixed-point in its renormalization group flow for the physical light-quark masses. An interesting line of investigation is the study of the scattering lengths as a function of the quark masses to ascertain the sensitivity of this fine-tuning to the QCD parameters [108, 109, 110]. The fine tuning is not expected to persist away from the physical masses and we expect present day (unphysical) Lattice QCD calculations to yield scattering lengths that are natural-sized. More generally, it is interesting to determine how the structure of nuclei depends upon the fundamental constants of nature. In particular, we expect that any nuclear observable is essentially a function of only five constants, the length scale of the strong interactions, Λ_{QCD} , the quark masses, m_u , m_d and m_s , and the electromagnetic coupling α_e ²².

The first study of baryon-baryon scattering with Lattice QCD was performed more than a decade ago by Fukugita *et al* [111, 112]. This calculation was quenched and at relatively large pion masses, $m_\pi \gtrsim 550$ MeV. Since this time, the dependence of the NN scattering lengths upon the light-quark masses has been determined to various non-trivial orders in the EFT expansion [108, 109, 110], which is estimated to be valid up to $m_\pi \sim 350$ MeV. Therefore physical predictions of NN scattering parameters becomes possible with Lattice QCD calculations that are performed with pion masses less than ~ 350 MeV.

The NPLQCD collaboration performed the first $n_f = 2 + 1$ QCD calculations of nucleon-nucleon interactions [113] and hyperon-nucleon [114] interactions at low-energies but with unphysical pion masses, and the nucleon-nucleon scattering lengths were found to be of natural size. The fine-tunings at the physical values of the light-quark masses indicates that Lattice QCD calculations with quark masses much closer to the physical values (than today) are needed to extrapolate to the experimental values. The results of the Lattice QCD calculation at the lightest pion mass and the experimentally-determined scattering lengths at the physical value of the pion mass were used to constrain the chiral dependence of the scattering lengths from $m_\pi \sim 350$ MeV down to the chiral limit [113]. However, these results suggest various possible scenarios toward the chiral limit which can only be resolved by way of Lattice QCD calculations at lighter pion masses. In contrast, very little is known about the interactions between nucleons and hyperons from experiment, and Lattice QCD calculations can provide the best determinations of the corresponding scattering parameters and hence determine the role of hyperons in neutron stars.

The energy eigenstates in the finite lattice volume are classified by their global quantum numbers, baryon number, isospin, third component of isospin, strangeness, total momentum, and behavior un-

²²In the low-energy theory, the dependence on top, bottom and charm quark masses is encapsulated in Λ_{QCD} .

Table 2: Baryon-baryon channels calculated in Ref. [117].

Channel	I	I_z	s
pp (1S_0)	1	+1	0
np (3S_1)	0	0	0
$n\Lambda$ (1S_0)	$\frac{1}{2}$	$-\frac{1}{2}$	-1
$n\Lambda$ (3S_1)	$\frac{1}{2}$	$-\frac{1}{2}$	-1
$n\Sigma^-$ (1S_0)	$\frac{1}{2}$	$-\frac{3}{2}$	-1
$n\Sigma^-$ (3S_1)	$\frac{1}{2}$	$-\frac{3}{2}$	-1
$\Sigma^-\Sigma^-$ (1S_0)	2	-2	-2
$\Lambda\Lambda$ (1S_0)	0	0	-2
$\Xi^-\Xi^-$ (1S_0)	1	-1	-4

der hyper-cubic transformations. Six quark operators that are simple products of three-quark baryon operators are (generally) used as sources for the baryon-baryon correlation functions, but this is not a requirement. As a consequence, the baryon content of the interpolating operator is used to define the operator, e.g. $n\Lambda(^3S_1)$, but this operator will, in principle, couple to all states in the volume with the quantum numbers $B = 2$, $I = \frac{1}{2}$, $I_z = -\frac{1}{2}$, $s = -1$, and $^{2s+1}L_J = ^3S_1 + \dots$, where the ellipses denote states with higher total angular momentum that also project onto the A_1 irreducible representation of the cubic-group²³. Correlation functions for the nine baryon-baryon channels shown in Table 2 have been calculated, using both SS and SP correlators, as described in Ref. [115]. If the calculations were performed on gauge field configurations of infinite extent in the time-direction, so that only forward propagation could occur, some of the channels in Table 2 could be analyzed by considering contributions from a single scattering channel, e.g. NN , $\Xi^-\Xi^-$, $\Sigma^-\Sigma^-$, $n\Sigma^-$, for which a single, well-separated ground state with these quantum numbers is expected. However, other channels may require a multi-channel analysis, e.g. $n\Lambda$, $\Lambda\Lambda$. The $n\Lambda$ source will produce low-lying states in the lattice volume that are predominately linear combinations of the $n\Lambda$, $n\Sigma^0$ and $p\Sigma^-$ two-baryon states. The $\Lambda\Lambda$ source will produce low-lying states in the lattice volume that are predominately linear combinations of the $\Lambda\Lambda$, $\Sigma^{\pm,0}\Sigma^{\mp,0}$, and $N\Xi$ two-baryon states.

There are a number of ways to perform the statistical analysis of the correlation functions and determine the associated uncertainties. One way is to use the Jackknife method to determine the uncertainty in $p \cot \delta$ directly. However, this is complicated by the fact that $\mathbf{S}(x)$ in Eq. (32) is a singular function. An alternate method is to determine the value of p_n^2 and its associated uncertainty from the two-baryon energy splitting from Eq. (31), and then to propagate the central value and 1σ uncertainties through Eq. (31) to determine $p \cot \delta$.

An extensive exploration of the impact of high-statistics on one-, two- and three-baryon correlation functions on one ensemble of anisotropic clover gauge configurations generated by the Hadron Spectrum Collaboration was undertaken in Refs [74, 116, 117]. A total of $\gtrsim 440,000$ sets of calculations were performed using 1200 gauge configurations of size $20^3 \times 128$ with an anisotropy parameter $\xi = b_s/b_t =$

²³ The spatial dimensions of the gauge field configurations that have been used to date for such calculations are identical, and as such the eigenstates of the QCD Hamiltonian can be classified with respect to their transformation properties under cubic transformations, $H(3)$, a subgroup of the group of continuous three-dimensional rotations, $O(3)$. The two-baryon states that are calculated in this work all belong to the A_1^+ representation of $H(3)$, corresponding to states with angular momentum $L = 0, 4, 6, \dots$.

3.5, a spatial lattice spacing of $b_s = 0.1227 \pm 0.0008$ fm, and pion mass of $M_\pi \sim 390$ MeV. The ground state baryon masses (in lattice units) were extracted with uncertainties that are at or below the $\sim 0.2\%$ -level. Figure 13 shows the effective $|\mathbf{k}|^2$ plot for both the proton-proton and neutron-proton channels. Both channels exhibit plateaus in $|\mathbf{k}|^2$. While the plateau in the proton-proton channel differs from zero

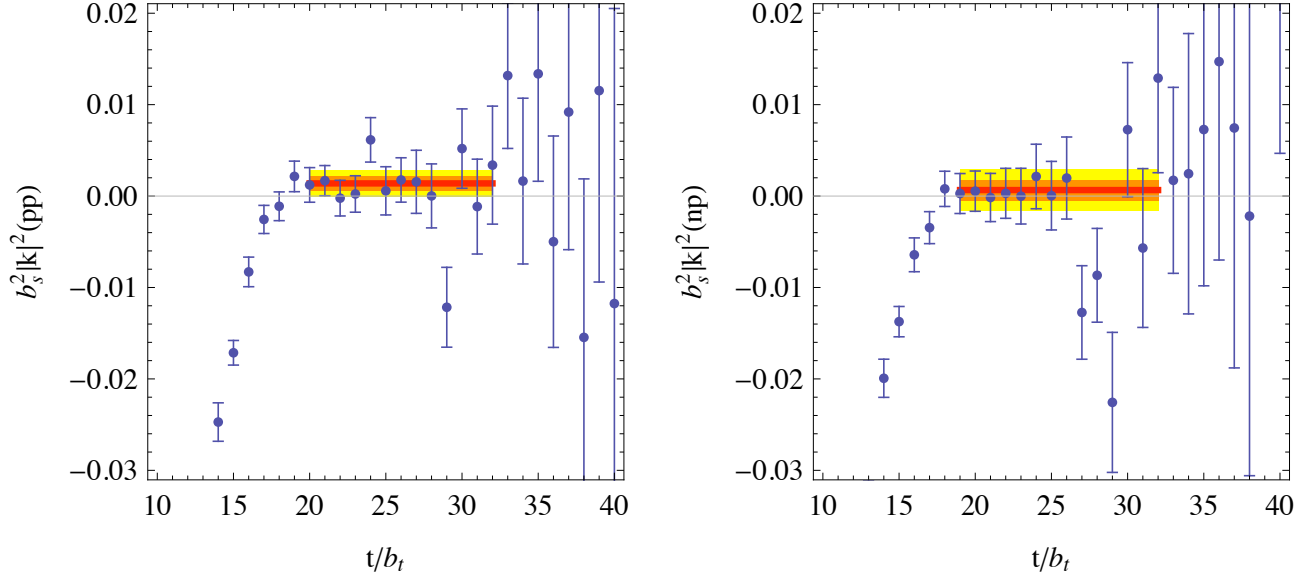


Figure 13: The left (right) panel is the effective $|\mathbf{k}|^2$ plot for the proton-proton (1S_0) (neutron-proton (3S_1)) channel and the fit to the plateau for the calculations on anisotropic clover gauge configurations in Ref. [117].

at the $\sim 1\text{-}\sigma$ level, the plateaus in both channels are consistent with zero. We conclude that at this value of the pion mass, the interactions between nucleons produce a small scattering length in both channels compared to the naive estimate of $m_\pi^{-1} \sim 0.5$ fm. A summary of all Lattice QCD calculations of NN scattering is shown in Figure 14. The results calculated on the anisotropic clover gauge configurations are consistent with those obtained with mixed-action Lattice QCD [113]. It is interesting to note that the results of quenched calculations [118] yield scattering lengths that are consistent within uncertainties with the fully-dynamical $n_f = 2 + 1$ values. Figure 15 shows a summary of the high-statistics results for baryon-baryon interactions obtained on the anisotropic clover gauge configurations. The $\Lambda\Lambda$ channel is found to be negatively shifted in energy which may signal that the lowest-state is in fact a bound-state, but calculations in a larger volume are required before more definitive conclusions can be drawn. The calculations constitute an order of magnitude jump forward in the volume of output for this type of calculation. The two additional lattice volumes in which we are presently performing calculations at this pion mass will allow for a systematic exploration of the volume dependence of the scattering amplitude for all of the two-hadron systems. In principle, this will enable a separation of scattering and bound states. However, calculations at this pion mass should be viewed to be only a proof of principle and a testing ground for new analysis techniques. In order for lattice calculations to provide meaningful constraints on interactions at the physical pion mass through chiral extrapolation, the pion mass must be substantially reduced down toward the physical value ($m_\pi \sim 140$ MeV) while maintaining the integrity of the calculation (i.e. small enough lattice spacings and large enough volumes).

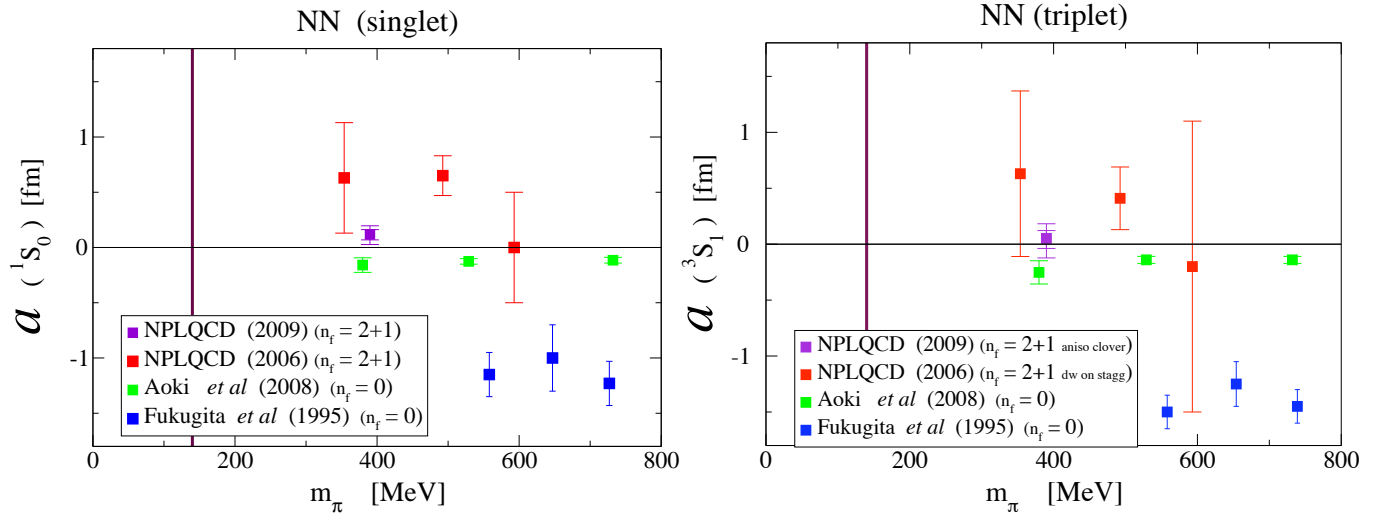


Figure 14: A compilation of the scattering lengths for NN scattering in the 1S_0 (left panel) and 3S_1 (right panel) calculated with Lattice QCD and with quenched Lattice QCD. The vertical lines correspond to the physical pion mass.

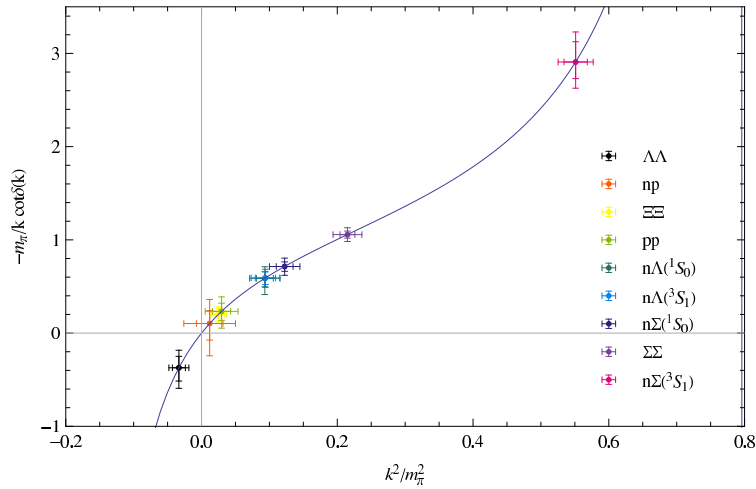


Figure 15: Baryon-baryon interactions extracted from calculations at $m_\pi \sim 390$ MeV and in a lattice volume of $20^3 \times 128$ [117]. The top-most point of the plot-legend corresponds to the left-most point on the plot, and the bottom-most point of the plot-legend corresponds to the right-most point on the plot. The other points are ordered accordingly.

4 Few-Body Physics

Computing resources and lattice algorithms have reached a stage where it is now possible to consider more complicated hadronic observables such as those in the baryon number, $B > 2$ sector — the domain of nuclei. Here there are many observables about which very little (or nothing) is known experimentally or theoretically, but which are phenomenologically important to nuclear structure and interactions and to nuclear astrophysics. Systems containing more than two mesons are of phenomenological interest in a number of areas from heavy ion collisions at RHIC, to the equation of state of neutron stars. In the last few years, there has been a concerted effort to understand and develop the techniques needed for

studying systems of a few or many hadrons.

4.1 Multi-Meson Interactions

As discussed previously, it has been known for many years how to exploit the volume dependence of the eigen-energies of two-hadron systems to extract infinite volume scattering phase shifts [78] provided that the effective range of the interaction, r is small compared to the spatial extent of the lattice volume (since $r \sim m_\pi^{-1}$ for most interactions, this constraint is $m_\pi L \gg 1$). In recent works, this has been extended to systems involving $n > 2$ bosons [119, 120, 121] and $n = 3$ fermions [122] in the situation where the relevant scattering length, a , is small compared to the spatial extent of the lattice. By performing a perturbative EFT calculation in a finite volume, the ground state energy of a system of n bosons was computed in Refs. [119, 120, 121]. The shift in energy of n bosons of mass M from the non-interacting system is

$$\begin{aligned} \Delta E_n = & \frac{4\pi \bar{a}}{M L^3} {}^nC_2 \left\{ 1 - \left(\frac{\bar{a}}{\pi L} \right) \mathcal{I} + \left(\frac{\bar{a}}{\pi L} \right)^2 [\mathcal{I}^2 + (2n-5)\mathcal{J}] \right. \\ & - \left(\frac{\bar{a}}{\pi L} \right)^3 [\mathcal{I}^3 + (2n-7)\mathcal{I}\mathcal{J} + (5n^2 - 41n + 63)\mathcal{K}] \\ & + \left(\frac{\bar{a}}{\pi L} \right)^4 [\mathcal{I}^4 - 6\mathcal{I}^2\mathcal{J} + (4+n-n^2)\mathcal{J}^2 + 4(27-15n+n^2)\mathcal{I}\mathcal{K} \\ & \left. + (14n^3 - 227n^2 + 919n - 1043)\mathcal{L}] \right\} \\ & + {}^nC_3 \left[\frac{192 \bar{a}^5}{M\pi^3 L^7} (\mathcal{T}_0 + \mathcal{T}_1 n) + \frac{6\pi \bar{a}^3}{M^3 L^7} (n+3) \mathcal{I} \right] \\ & + {}^nC_3 \frac{1}{L^6} \bar{\eta}_3^L + \mathcal{O}(L^{-8}) \quad , \end{aligned} \quad (50)$$

where the parameter \bar{a} is related to the scattering length, a , and the effective range, r , by

$$a = \bar{a} - \frac{2\pi}{L^3} \bar{a}^3 r \left(1 - \left(\frac{\bar{a}}{\pi L} \right) \mathcal{I} \right) \quad . \quad (51)$$

The geometric constants, \mathcal{I} , \mathcal{J} , \mathcal{K} , \mathcal{L} , $\mathcal{T}_{0,1}$, that enter into Eq. (50) are defined in Ref. [121] and nC_m are the binomial coefficients. The three-body contribution to the energy-shift given in Eq. (50) is represented by the parameter $\bar{\eta}_3^L$ (see Ref. [121]).

Lattice QCD calculations of these energy shifts allow for an extraction of the parameters \bar{a} and $\bar{\eta}_3^L$. To determine the energy shifts, the multi-meson correlation functions (specifying to the multi-pion system)

$$C_n(t) \propto \left\langle \left(\sum_{\mathbf{x}} \pi^-(\mathbf{x}, t) \right)^n \left(\pi^+(\mathbf{0}, 0) \right)^n \right\rangle \quad , \quad (52)$$

are calculated. On a lattice of infinite temporal extent,²⁴ the combination

$$G_n(t) \equiv \frac{C_n(t)}{[C_1(t)]^n} \xrightarrow{t \rightarrow \infty} \mathcal{B}_0^{(n)} e^{-\Delta E_n t} \quad , \quad (53)$$

²⁴Effects of temporal (anti-)periodicity are discussed in Ref. [123].

allows for an extraction of the ground-state energy shift, ΔE_n , which can then be used as input into Eq. (50) to extract the scattering and interaction parameters. To compute the $(n!)^2$ Wick contractions in Eq. (52), the correlation function can be written as

$$C_n(t) \propto \langle (\bar{\eta} \Pi \eta)^n \rangle \propto \varepsilon^{\alpha_1 \alpha_2 \dots \alpha_n \xi_1 \dots \xi_{12-n}} \varepsilon_{\beta_1 \beta_2 \dots \beta_n \xi_1 \dots \xi_{12-n}} (\Pi)_{\alpha_1}^{\beta_1} (\Pi)_{\alpha_2}^{\beta_2} \dots (\Pi)_{\alpha_n}^{\beta_n} ,$$

$$\Pi = \sum_{\mathbf{x}} S(\mathbf{x}, t; 0, 0) S^\dagger(\mathbf{x}, t; 0, 0) , \quad (54)$$

where $S(\mathbf{x}, t; 0, 0)$ is a light-quark propagator. The object (block) Π is a $N \times N$ bosonic time-dependent matrix where $N = 12$ ($N = N_S \times N_C$ with $N_S = 4$ -spin and $N_C = 3$ -color), and η_α is a twelve component Grassmann variable. Further simplifications are possible resulting in the correlation functions being written in terms of traces of powers of Π . As an example, the contractions for the $3\text{-}\pi^+$ system give

$$C_3(t) \propto \text{tr}_{\text{C,S}} [\Pi]^3 - 3 \text{tr}_{\text{C,S}} [\Pi^2] \text{tr}_{\text{C,S}} [\Pi] + 2 \text{tr}_{\text{C,S}} [\Pi^3] , \quad (55)$$

where the traces, $\text{tr}_{\text{C,S}}$, are over color and spin indices. Contractions for $n \leq N$ π^+ 's are given explicitly in Ref. [124].

4.2 Two- and Three- Body Interactions

The NPLQCD collaboration has performed mixed-action Lattice QCD calculations of the $n \leq 12$ pion and kaon correlation functions [123, 124, 125]. In order to correctly calculate these correlators for large n , very high numerical precision is necessary and the ARPREC arbitrary precision numerical library [126] was used. By performing a correlated fit to the effective energy differences extracted from these calculations, the two- and three-body interactions were determined [123, 124, 125], and the two-body interactions agree with those extracted from the two-body sector alone [95]. The resulting three-body interactions are displayed in Figure 16. The $3\text{-}\pi^+$ interaction is found to be repulsive with a magnitude consistent with the expectation from naive dimensional analysis (tree-level χ -PT). In contrast, the three K^+ interaction is consistent with zero within somewhat larger uncertainties.

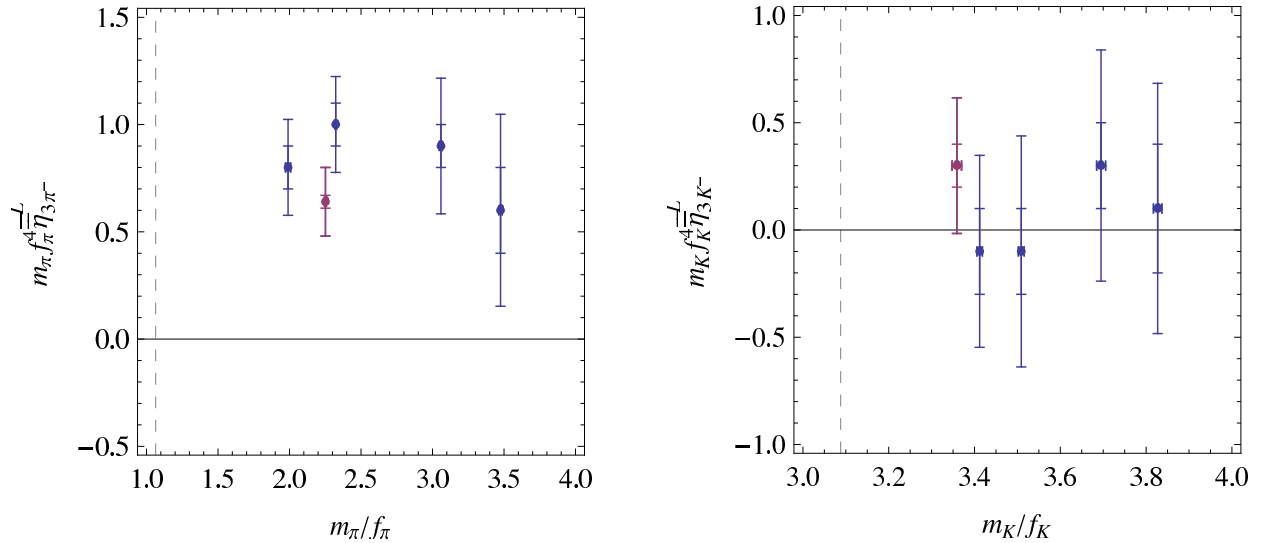


Figure 16: Three pion (left-panel) and kaon (right-panel) interactions determined from the MILC coarse (lighter, blue) and fine (darker, magenta) lattices plotted as a function of the dimensionless ratios m_π/f_π and m_K/f_K respectively.

4.3 Mixed Species Meson Systems

In the case of a mixed system comprising n mesons of one type and m mesons of a second type, the results summarized in Section 4.1 have been generalized by Smigielski and Wasem [127], working to $\mathcal{O}(1/L^6)$. The energy shift of the interacting system from the free system depends on three two-body interaction parameters and four three-body interaction parameters. As might be expected, the full form of the energy shift is cumbersome and we refer the interested reader to the original paper. These expressions are currently being used to analyze LQCD calculations of the energies of systems of pions and kaons [128]. Correlation functions are calculated in a way that is similar to the way that the multi-pion correlation functions are calculated.

4.4 Contractions for Large ($N > 12$) Systems of Mesons

In order to go beyond $n = 12$ meson systems, or to study systems of many different types of mesons, it is necessary to make use of more efficient methods of performing the contractions of quark fields. While better than the naïve factorial construction (which scales as $n!$), the construction used in Section 4.1 scales poorly to large numbers of mesons, behaving at best as $n!^{1/2}$ (provided the matrix Π is generalized to give a nonzero result). In Ref. [129], a recursive method for performing these contractions was developed that allows the extension of the study of meson systems to larger n and also greatly simplifies the contractions required for systems of many different species of mesons. We will summarize the construction by first considering the recursive approach to the contractions for a single species of meson before reporting the general case.

By rescaling the correlation functions of the single-species, single-source system considered previously as

$$C_{n\pi^+}(t) = (-)^n n! \langle R_n \rangle, \quad (56)$$

(the angle brackets denote a trace over spin and color indices) it is straightforward to show that the objects, R_n satisfy an ascending recursion

$$R_{n+1} = \langle R_n \rangle \Pi - n R_n \Pi. \quad (57)$$

with the initial condition that $R_1 = \Pi$ as defined in Eq. (54). To see how this works we explicitly construct the first few terms:

$$\begin{aligned} R_2 &= \langle R_1 \rangle \Pi - R_1 \Pi = \langle \Pi \rangle \Pi - \Pi^2 \\ \langle R_2 \rangle &= \langle \Pi \rangle^2 - \langle \Pi^2 \rangle, \\ R_3 &= \langle R_2 \rangle \Pi - 2 R_2 \Pi = \langle \Pi \rangle^2 \Pi - \langle \Pi^2 \rangle \Pi - 2 \langle \Pi \rangle \Pi^2 + 2 \Pi^3 \\ \langle R_3 \rangle &= \langle \Pi \rangle^3 - 3 \langle \Pi^2 \rangle \langle \Pi \rangle - 2 \langle \Pi^3 \rangle, \end{aligned} \quad (58)$$

in agreement with Eq. (55). Descending recursions also exist.

A correlation function for a system composed of n_{ij} mesons of the i^{th} species from the j^{th} source at $(\mathbf{y}_j, 0)$, where $0 \leq i \leq k$ and $0 \leq j \leq m$, is of the form

$$\begin{aligned} C_{\mathbf{n}}(t) &= \left\langle \left(\sum_{\mathbf{x}} \mathcal{A}_1(\mathbf{x}, t) \right)^{\mathcal{N}_1} \dots \left(\sum_{\mathbf{x}} \mathcal{A}_k(\mathbf{x}, t) \right)^{\mathcal{N}_k} \right. \\ &\quad \left. \left(\mathcal{A}_1^\dagger(\mathbf{y}_1, 0) \right)^{n_{11}} \dots \left(\mathcal{A}_1^\dagger(\mathbf{y}_m, 0) \right)^{n_{1m}} \dots \left(\mathcal{A}_k^\dagger(\mathbf{y}_1, 0) \right)^{n_{k1}} \dots \left(\mathcal{A}_k^\dagger(\mathbf{y}_m, 0) \right)^{n_{km}} \right\rangle, \end{aligned} \quad (59)$$

where $\mathcal{N}_i = \sum_j n_{ij}$ is the total number of mesons of species i , and the subscript in $C_{\mathbf{n}}(t)$ labels the number of each species from each source,

$$\mathbf{n} = \begin{pmatrix} n_{11} & n_{12} & \dots & n_{1m} \\ \vdots & \vdots & \vdots & \vdots \\ n_{k1} & n_{k2} & \dots & n_{km} \end{pmatrix} . \quad (60)$$

The $\mathcal{A}_i(\mathbf{y}, t)$ denotes a quark-level interpolating operator $\mathcal{A}_m(\mathbf{x}, t) = \bar{q}_m(\mathbf{x}, t) \gamma_5 u(\mathbf{x}, t)$, and it is straightforward to show that [129]

$$C_{\mathbf{n}}(t) = \left(\prod_i \mathcal{N}_i! \right) \left\langle \prod_{i,j} (\bar{\eta} P_{ij} \eta)^{n_{ij}} \right\rangle = (-)^{\bar{\mathcal{N}}} \frac{(\prod_i \mathcal{N}_i!) (\prod_{i,j} n_{ij}!)}{\bar{\mathcal{N}}!} \langle T_{\mathbf{n}} \rangle , \quad (61)$$

where the η are $m \times N$ -component Grassmann variables, and the P_{ij} are $\bar{N} \times \bar{N}$ dimensional matrices, where $\bar{N} = m \times N$, which are generalizations of the Π defined in Eq. (54) with an additional species index, i . They are defined as

$$P_{ij} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ (A_i)_{j1}(t) & (A_i)_{j2}(t) & \dots & (A_i)_{jm}(t) \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix} , \quad (A_i)_{ab} = \sum_{\mathbf{x}} S(\mathbf{x}, t; \mathbf{y}_b, 0) S_i^\dagger(\mathbf{x}, t; \mathbf{y}_a, 0) , \quad (62)$$

The $(A_i)_{ab}$ are $N \times N$ dimensional matrices, one for each flavor, i , and pair of source indices, a and b . $\bar{\mathcal{N}} = \sum_i \mathcal{N}_i$ is the total number of mesons in the system, with $\bar{\mathcal{N}} \leq \bar{N}$. The $T_{\mathbf{n}}$ defined implicitly in Eq. (61) satisfy the recursion relation

$$T_{\mathbf{n}+\mathbf{1}_{rs}} = \sum_{i=1}^k \sum_{j=1}^m \langle T_{\mathbf{n}+\mathbf{1}_{rs}-\mathbf{1}_{ij}} \rangle P_{ij} - \bar{\mathcal{N}} T_{\mathbf{n}+\mathbf{1}_{rs}-\mathbf{1}_{ij}} P_{ij} , \quad (63)$$

where

$$\mathbf{1}_{ij} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix} , \quad (64)$$

and where the non-zero value is in the $(i, j)^{\text{th}}$ entry. Defining $\mathcal{U}_j = \sum_i n_{ij}$ to be the number of mesons from the j^{th} source, it is clear that the correlation function vanishes when $\mathcal{U}_j > N$ for any source j .

These recursion relations (and those for the simpler systems also studied in Ref. [129]) allow for the calculation of arbitrarily large systems of mesons. As formulated above, the systems are restricted to contain quarks of one flavor but anti-quarks of any number of flavors²⁵ or vice versa. Importantly the above algorithm scales linearly with the total number of mesons in the system.

²⁵This restriction is not necessary, but relaxing it results in much more complex sets of recursions.

4.5 Pion and Kaon Condensation

The ground state of a generic system of many bosons with repulsive interactions is a Bose-condensed phase. The QCD systems of pions or kaons discussed above form a Bose-Einstein condensate of fixed third-component of isospin, I_z , and strangeness, s . It is of significant theoretical and phenomenological interest to investigate the properties of such systems. Theoretical efforts have used LO χ -PT to investigate the phase diagram at low chemical potential [130] and it is important to assess the extent to which these results agree with QCD. In neutron stars, it is possible that it is energetically favorable to (partially-) neutralize the system with a condensate of K^- mesons, and an isospin chemical potential resulting from the isospin asymmetry of the colliding nuclei may play an important role in the study of the QCD phase diagram at RHIC. Numerical calculations provide a probe of the dependence of the energy on the pion or kaon density, and thereby allow for an extraction of the chemical potential via a finite difference. The results from mixed-action calculations are shown in Figure 17 and Figure 18. Also shown are the predictions of tree-level χ -PT, which are in remarkably good agreement. This is encouraging for studies of kaon condensation in neutron stars where, typically, tree level χ -PT interactions amongst kaons, and between kaons and baryons [101], are assumed.

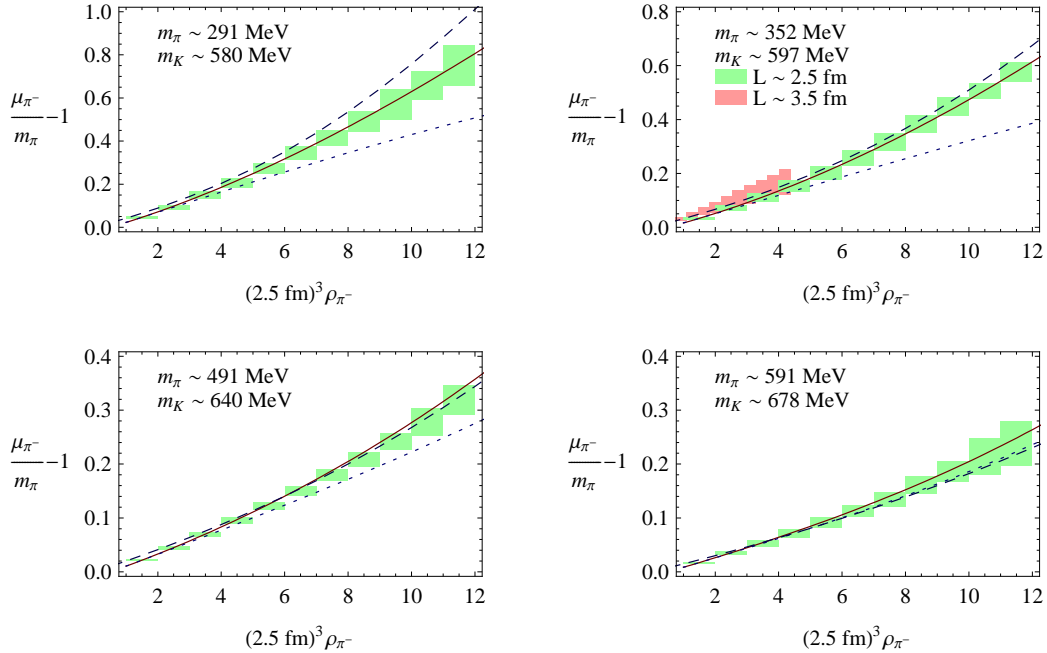


Figure 17: The dependence of the isospin chemical potential on the pion density. The curves correspond to the predictions of tree level χ -PT (dashed) [130], the energy shift of Eq. (50) (solid) and without the three-body interaction (dotted).

4.6 Hadronic Medium Effects

The hadronic medium formed in the multi-meson calculations described above is naturally expected to influence the properties of other hadrons that interact with it. A phenomenologically relevant example is the passage of a J/Ψ meson through medium as J/Ψ suppression is taken to be a key signal for the formation of a new state of matter at high temperatures, such as the quark-gluon plasma [131]. In Ref. [132], a simplified version of this scenario was considered, and the screening of the static quark potential (the potential between an infinitely massive quark-anti-quark pair) by a Bose-Einstein condensate of π^+ 's was computed. In order to extract the shift in the static potential caused by the presence

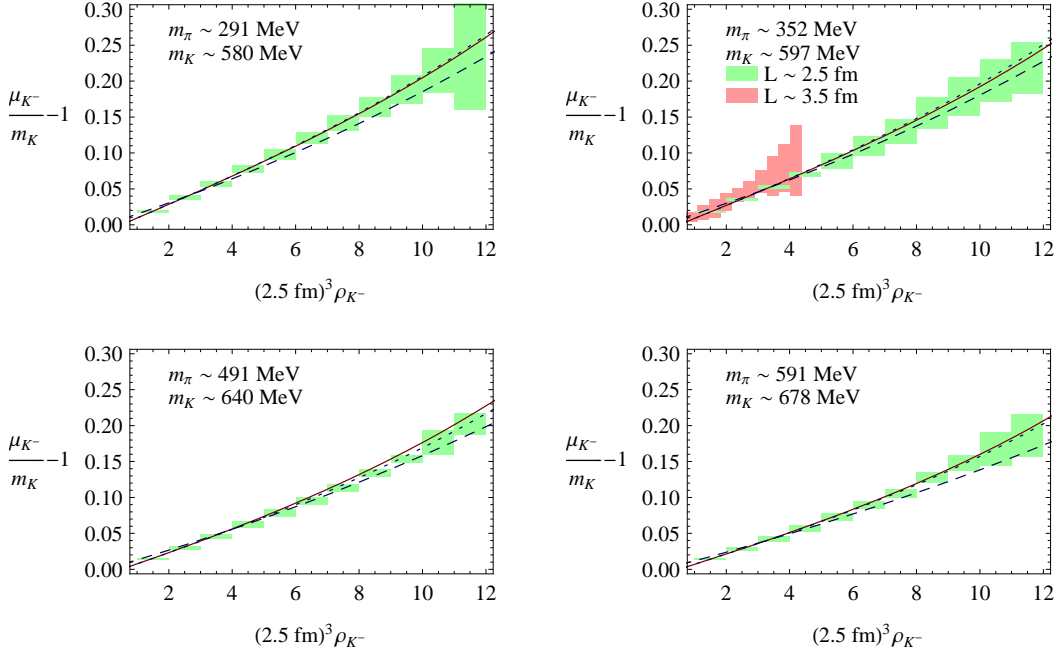


Figure 18: The dependence of the strangeness chemical potential on the kaon density. The curves correspond to the predictions of tree level chiral perturbation theory (dashed) [130], the energy shift of Eq. (50) (solid) and without the three-body interaction (dotted).

of the medium, the following ratio of correlation functions was calculated

$$G_{n,W}(R, t_\pi, t_w, t) = \frac{C_{n,W}(R, t_\pi, t_w, t)}{C_n(t_\pi, t) C_W(R, t_w, t)} , \quad (65)$$

where C_n is defined in Eq. (52) and

$$C_W(R, t_w, t) = \left\langle 0 \left| \sum_{\mathbf{y}, |\mathbf{r}|=R} \mathcal{W}(\mathbf{y} + \mathbf{r}, t; \mathbf{y}, t_w) \right| 0 \right\rangle ,$$

$$C_{n,W}(R, t_\pi, t_w, t) = \left\langle 0 \left| \left[\sum_{\mathbf{x}} \pi^-(\mathbf{x}, t) \pi^+(0, t_\pi) \right]^n \sum_{\mathbf{y}, |\mathbf{r}|=R} \mathcal{W}(\mathbf{y} + \mathbf{r}, t; \mathbf{y}, t_w) \right| 0 \right\rangle , \quad (66)$$

and $\mathcal{W}(\mathbf{y}, t_0; \mathbf{y} + \mathbf{r}, t)$ is the Wilson-loop operator formed from products of gauge links joining the vertices at (\mathbf{y}, t_0) , $(\mathbf{y} + \mathbf{r}, t_0)$, $(\mathbf{y} + \mathbf{r}, t)$ and (\mathbf{y}, t) . At large Euclidean time, this ratio falls exponentially with a scale $\delta V(R, n)$ that is the shift in static potential for separation $R = |\mathbf{r}|$ and isospin density $\rho = \rho_0 n$ (where $\rho_0 = 1/V \sim 0.064 \text{ fm}^{-3}$). Further details are discussed in Ref. [132].

As expected from the weak nature of pion interactions with isoscalar objects, the overall screening effect is small. In the region where the force between the static quark and anti-quark is constant, $F \sim 1 \text{ GeV fm}^{-1}$, the shift is $\mathcal{O}(\text{MeV fm}^{-1})$. The shift in the force was found to vary linearly with the isospin density of the hadronic system as shown in Figure 19. This is consistent with a simple interpretation in terms of a dielectric in the volume of the color flux tube between the quark-anti-quark pair. Further calculations extending this study to dynamical charm quarks are underway. To directly connect with phenomenology, the more difficult problem of finite baryon density must be confronted.

4.7 Three-Baryon Systems

The first significant steps towards the calculation of the properties of nuclei directly from QCD were taken by the NPLQCD collaboration [116] and the PACS-CS collaboration [133] during 2009. The

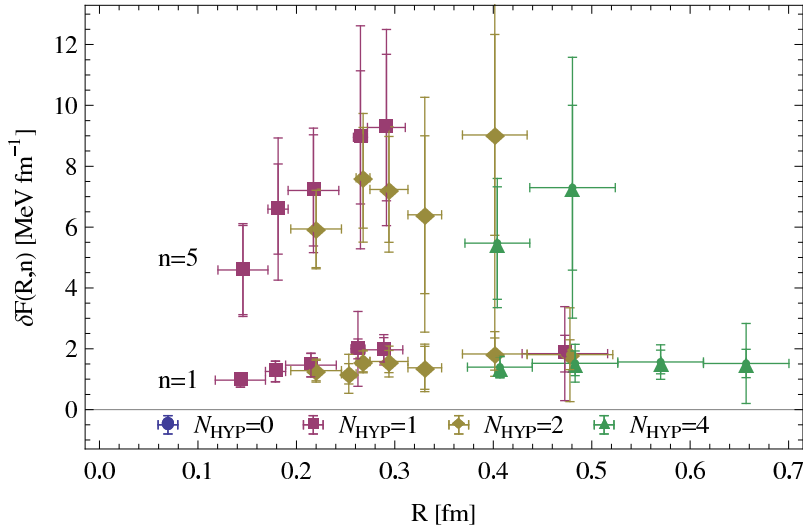


Figure 19: The in-medium contribution to the radial $Q\bar{Q}$ force, $\delta F(R, n)$, at a pion number density of ρ_0 and $5\rho_0$. The inner uncertainty associated with each point is statistical, while the outer is the statistical and systematic uncertainties combined in quadrature.

NPLQCD collaboration performed a $n_f = 2+1$ calculation of the correlation function with the quantum numbers of the strangeness $s = -4$, baryon number $B = 3$ system, which is labeled as “ $n\Xi^0\Xi^0$ ” for convenience, and also of the correlation function with the quantum numbers of the triton (or ${}^3\text{He}$), at a pion mass of $m_\pi \sim 390$ MeV [116]. Further, the PACS-CS collaboration performed a quenched calculation of the system with the quantum numbers of the triton and of the α -particle at a pion mass of $m_\pi \sim 800$ MeV [133].

The NPLQCD collaboration calculation used the product of single baryon sources and sinks for the source and sink of the three-baryon correlation functions. In the $n\Xi^0\Xi^0$ -channel they were the product of two Ξ and one nucleon source or sink, with the spin quantum numbers constructed to produce a state with total $J = 0$ and third component of isospin $I_z = \frac{1}{2}$. In the triton channel, the product of three nucleon interpolating operators were used to construct an operator with $J = \frac{1}{2}$ and with total isospin $I = \frac{1}{2}$. The correlation function in the $n\Xi^0\Xi^0$ -channel, shown in Figure 20, yields an energy-splitting that is consistent with zero within the uncertainties of the calculation, as shown in Figure 21,

$$\delta E_{\Xi^0\Xi^0 n} = 4.6 \pm 5.0 \pm 7.9 \pm 4.2 \text{ MeV} \quad , \quad \chi^2/\text{dof} = 2.0 \quad , \quad (67)$$

It is very encouraging that the uncertainty in the energy-shift per baryon is ~ 3 MeV, which is smaller than the binding-energy per nucleon in typical nuclei, $B \sim 8$ MeV, and not significantly larger than the binding-energy per nucleon in the deuteron or triton at the physical values of the light-quark masses. The single energy-level fit to the EMP in Figure 21 has a $\chi^2/\text{dof} = 2.0$, indicating that there may be additional structure in the correlation function. Including a second energy-level shifted by $\Delta E \sim -0.004$ lattice units might provide a better description of the EMP, and would be consistent with the lower-energy state, $\Xi^0\Lambda\Lambda$, that is expected to contribute to the four low-lying eigenstates in the lattice-volume. However, enhanced statistics are required to determine if this is, in fact, the case.

At present, unlike the situation in multi-meson systems [125, 124, 123], the analytical tools are not in place to use the above energy shift and those of the associated two-baryon systems to extract the parameters describing the relevant two- and three-body interactions. While the volume dependence of the simplest three-fermion systems has been studied in Ref. [122], the mixing we expect between four closely spaced states significantly complicates the situation.

The NPLQCD collaboration focused on the state(s) that couples to the $\Xi^0\Xi^0 n$ interpolating-operator simply due to limited computational resources and the expectation that the large strange quark content

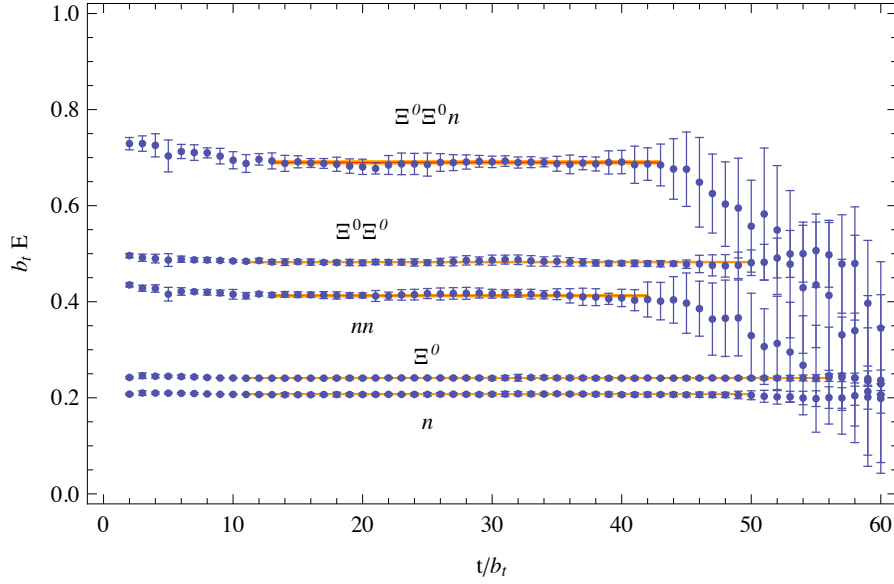


Figure 20: The EMPs for the nucleon, Ξ , nn , $\Xi^0 \Xi^0$ and $n \Xi^0 \Xi^0$ systems obtained by the NPLQCD collaboration [116].

would lead to a clean signal. In the past it has been the case that gauge field generation has required the majority of LQCD resources, but this is no longer true for precise calculations of baryonic observables. The resources that are presently required to perform the large number of calculations required for nuclear systems is significantly greater than that required for gauge field generation. This situation will improve as more effort is put into algorithmic improvements for contractions, in the same way that the use of deflation and other techniques have greatly reduced the resources required for propagator generation. Work in this direction is in progress. Given the observed behavior of the signal-to-noise ratio, which will be discussed in Section 5, identification of the ground state in systems of four and five baryons is anticipated in the near future.

The number of contractions that must be performed in order to calculate the correlation function in the triton channel is significantly greater than the number in the $\Xi^0 \Xi^0 n$, and therefore a smaller number of contractions was possible with the computational resources available to NPLQCD. The results of the

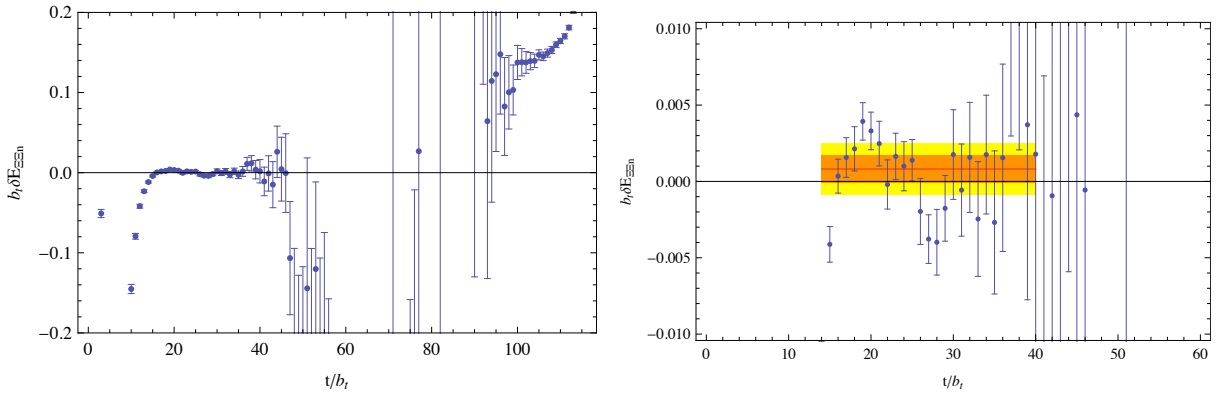


Figure 21: The EMP of the difference between the energy of the $n \Xi^0 \Xi^0$ channel and its constituent hadrons [116]. The right panel is an enlargement of part of the left panel.

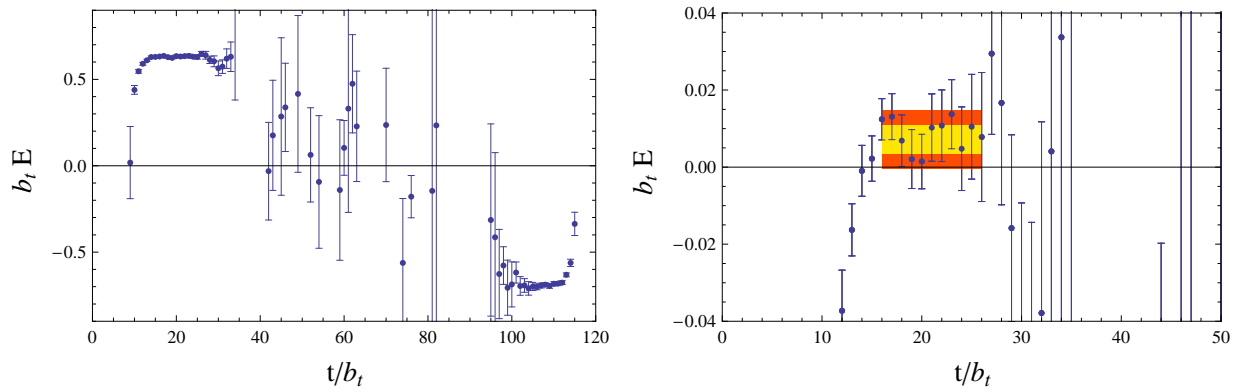


Figure 22: The EMP for the correlation function with the quantum numbers of the triton (left panel), and for the difference between the triton and its constituents (right panel) [116].

calculations performed by the NPLQCD collaboration of the correlation function in the channel with the quantum numbers of the triton are shown in Figure 22. A clear plateau is found for the ground-state of the system in the lattice volume in the window of time-slices where the signal-to-noise ratio is not degrading exponentially. However, the uncertainty remains too large to determine if the ground state corresponds to a positively or negative shifted state,

$$\delta E_{pnn} = 40 \pm 21 \pm 38 \text{ MeV} , \quad \chi^2/\text{dof} = 0.97 , \quad (68)$$

corresponding to ~ 13 MeV-per-baryon. However, the fact that a plateau in the triton channel has been observed at a relatively light pion mass ($m_\pi \sim 390$ MeV) is a very encouraging step forward.

Unfortunately, none of the calculations that have been performed to date for systems of three or more baryons have managed to calculate energy-shifts that exceed $5\text{-}\sigma$ deviations from zero, and, as such, compelling calculations are yet to be performed. However, such calculations are expected in the near future.

At the physical pion mass, the expected energy eigenvalues of two nucleons in a lattice volume with $m_\pi L \gg 1$ have been determined [82]. Recently, there have been efforts undertaken to determine the expected energy eigenvalues of systems composed of three nucleons [122, 134, 135, 136, 137] in cubic volumes with periodic boundary conditions using EFT. It is found that the triton binding energy is less sensitive to a finite-volume than the deuteron binding energy, which can be understood in terms of the spatial extent of the respective wavefunctions. These works are the beginning of a series of theoretical calculations that should be performed to provide a guide in determining the Lattice QCD calculations that should be performed to best extract the parameters in the EFT which will then allow for a description of more complex processes of relevance to nuclear physics.

4.8 Four-Baryon Interaction

In late 2009, the PACS-CS collaboration performed the first quenched calculation of a four-baryon correlation function [133] in the channel that will contain the α -particle (${}^4\text{He}$ nucleus) when performed at the physical pion mass. The pion mass used in these calculations is large, $m_\pi \sim 800$ MeV, and sea quark effects are ignored. Nonetheless this is a very important step towards calculating the properties and interactions of nuclei. The PACS-CS collaboration results are shown in Figure 23. One hopes to see significantly improved statistics in the near future for such an important quantity.

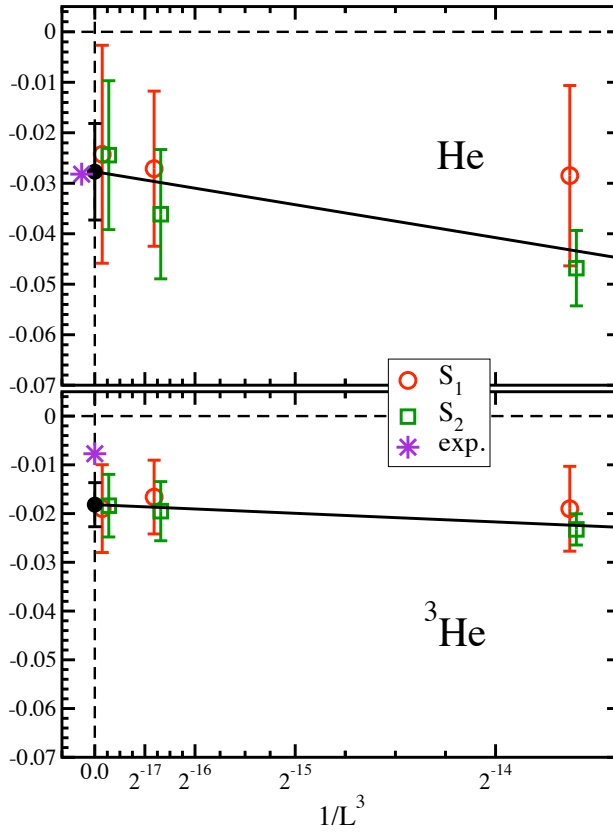


Figure 23: The quenched results for the binding energies (in lattice units) obtained by the PACS-CS collaboration in the triton channel and the channel with the quantum numbers of the α -particle [133]. The pion mass in these calculations is $m_\pi \sim 800$ MeV.

5 The Signal-to-Noise Ratio in Baryon Correlation Functions

Until recently it had been lore that the signal-to-noise ratio in baryon correlation functions degrades exponentially with the baryon number. The correlation functions exhibit this behavior at large times [138], and if this were the only part of the correlation functions that could be calculated with precision, the calculation of quantities of importance to nuclear physics would require exponentially more computing resources than those of importance to particle physics. However, during the last year it has been realized that such exponential degradation of the signal-to-noise ratio is absent at intermediate times over an interval that is dictated by the structure of the source and sink of the correlation function [115, 116, 117]. A consequence of this behavior is that it is possible to extract information about multi-baryon systems where the only additional computational resources required are those to perform the contractions.

In the case of a source that has the quantum numbers of a single positive parity nucleon, the correlation function on an ensemble of gauge field configurations with infinite temporal extent has the form [138]

$$\langle \theta_N(t) \rangle = \sum_{\mathbf{x}} \Gamma_+^{\beta\alpha} \langle 0 | N^\alpha(\mathbf{x}, t) \bar{N}^\beta(\mathbf{0}, 0) | 0 \rangle \rightarrow Z_N e^{-M_N t} , \quad (69)$$

where $N^\alpha(\mathbf{x}, t)$ is an interpolating field (composed of three quark operators) that has non-vanishing overlap with the nucleon, Γ_+ is a positive energy projector, and the angle brackets indicate statistical averaging over calculations on an ensemble of configurations. The variance of this correlation function

is given by

$$\begin{aligned}
N \sigma^2 &\sim \langle \theta_N^\dagger(t) \theta_N(t) \rangle - \langle \theta_N(t) \rangle^2 \\
&= \sum_{\mathbf{x}, \mathbf{y}} \Gamma_+^{\delta\alpha} \Gamma_+^{\gamma\beta\dagger} \langle 0 | N^\alpha(\mathbf{x}, t) \bar{N}^\beta(\mathbf{y}, t) N^\gamma(\mathbf{0}, 0) \bar{N}^\delta(\mathbf{0}, 0) | 0 \rangle - \langle \theta_N(t) \rangle^2 \\
&\rightarrow Z_{N\bar{N}} e^{-2M_N t} - Z_N^2 e^{-2M_N t} + Z_{3\pi} e^{-3m_\pi t} + \dots \xrightarrow{t \rightarrow \infty} Z_{3\pi} e^{-3m_\pi t} , \tag{70}
\end{aligned}$$

where all interaction energies have been neglected, and N is the number of (independent) calculations. At large times, the noise-to-signal ratio has the form, as argued by Lepage [138],

$$\frac{\sigma}{\bar{x}} = \frac{\sigma(t)}{\langle \theta(t) \rangle} \sim \frac{1}{\sqrt{N}} e^{(M_N - \frac{3}{2}m_\pi)t} . \tag{71}$$

More generally, for a system of A nucleons, the noise-to-signal ratio behaves as

$$\frac{\sigma}{\bar{x}} \sim \frac{1}{\sqrt{N}} e^{A(M_N - \frac{3}{2}m_\pi)t} \tag{72}$$

at large times.

The various “Z-factors”, such as $Z_{3\pi}$, depend upon the details of the sources and sinks interpolators that are used. For the calculations performed by the NPLQCD collaboration, the projection onto zero-momentum final state nucleons, introduces a $1/\sqrt{\text{Volume}}$ suppression of the amplitudes of the various components (except for $N\bar{N}$) in addition to color and spin rearrangement suppressions that exists independent of the spatial structure of the source. As a consequence, an interval of time slices exists at short times (the “Golden Window”) in which the variance of the correlation function is dominated by the terms in Eq. (71) that behave as $\sim e^{-2M_N t}$. In this window, the signal-to-noise ratio of the single baryon correlation function is independent of time. Further, the signal-to-noise ratio does not degrade exponentially faster in multi-baryon correlation functions than in single-baryon correlation functions in the “Golden Window”.

The finite temporal extent introduces backward propagating states (thermal states) into the correlation functions which lead to exponentially worse signal-to-noise ratios at large times [115, 116, 117]. These contributions are suppressed by at least $\exp(m_\pi T)$, however, they can cause complications. We note that the impact of these states can be mitigated by working at larger temporal extents and exponentially large computational resources are not required.

With the high statistics calculations that have been performed, the behavior of the signal-to-noise ratio has been carefully examined, and it was found to be useful to form the effective noise-to-signal plot [115]. On each time slice, the quantity

$$\mathcal{S}(t) = \frac{\sigma(t)}{\bar{x}(t)} , \tag{73}$$

is formed, from which the energy governing the exponential behavior (the signal-to-noise energy-scale) can be extracted via

$$E_{\mathcal{S}}(t; t_J) = \frac{1}{t_J} \log \left(\frac{\mathcal{S}(t + t_J)}{\mathcal{S}(t)} \right) . \tag{74}$$

For a correlation function that is dominated by a single state with a corresponding variance correlation function dominated by a single energy scale, the quantity $E_{\mathcal{S}}(t; t_J)$ will be independent of both t and t_J .

The signal-to-noise ratio in the one- and two-nucleon sector has the simplest structure as only up and down quarks appear in the interpolating operators. In the single nucleon sector, it is expected that

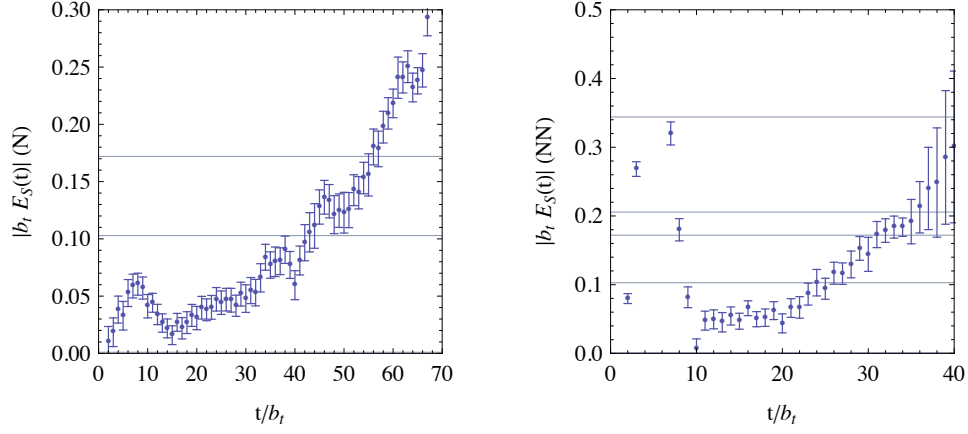


Figure 24: The energy scale of the signal-to-noise ratio in the nucleon (left panel) and proton-proton (right panel) correlation functions, defined in Eq. (74), obtained on $20^3 \times 128$ anisotropic clover gauge field configurations [115, 116, 117]. The horizontal lines in the left panel correspond to $E_s = 0$, $M_N - \frac{3}{2}m_\pi$ and $M_N - \frac{1}{2}m_\pi$, while those in the right panel correspond to $E_s = 0$, $M_N - \frac{3}{2}m_\pi$, $M_N - \frac{1}{2}m_\pi$, $2M_N - 3m_\pi$, $2M_N - m_\pi$.

the energy scales $E_S \sim 0$, $M_N - \frac{3}{2}m_\pi$, and others, contribute to the signal-to-noise ratio. At times when the nucleon correlation function is in the ground state, and the variance correlation function is dominated by the nucleon-antinucleon state, $E_S = 0$ should dominate the signal-to-noise ratio. At large times the variance correlation function is dominated by the 3-pion state and $E_S = M_N - \frac{3}{2}m_\pi$ should dominate. This is modified by the finite temporal direction [115] as the hadrons produced by the sources of the correlation function and the variance correlation function can propagate forward and backward in time. The calculated energy scale of the signal-to-noise ratio of the single nucleon correlation function obtained on $20^3 \times 128$ anisotropic clover gauge field configurations [115, 116, 117] is shown in Figure 24. It exhibits behavior that is consistent with expectations, and exceeds the long-time behavior expected from the Lepage argument at approximately time-slice $t = 50$ due to the temporal boundary conditions.

The structure of the two-nucleon variance correlation function has significantly more structure than that for one nucleon. On configurations with infinite temporal extent, the proton-proton correlation function is of the form (neglecting interactions between the hadrons)

$$\begin{aligned} \langle \theta_{NN}(t) \rangle &= \sum_{\mathbf{x}, \mathbf{y}} \Gamma_+^{\alpha\gamma\beta\rho} \langle 0 | N^\alpha(\mathbf{x}, t) N^\gamma(\mathbf{y}, t) \bar{N}^\beta(\mathbf{0}, 0) \bar{N}^\rho(\mathbf{0}, 0) | 0 \rangle \\ &\rightarrow Z_{NN} e^{-2M_N t} + \dots, \end{aligned} \quad (75)$$

and the variance correlation function has the form

$$\begin{aligned} \text{N } \sigma^2 &\sim \langle \theta_{NN}^\dagger(t) \theta_{NN}(t) \rangle - \langle \theta_{NN}(t) \rangle^2 \\ &= \sum_{\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w}} \Gamma_+^{\alpha\rho\delta\psi} \Gamma_+^{\beta\eta\gamma\zeta} \langle 0 | N^\alpha(\mathbf{x}, t) N^\rho(\mathbf{y}, t) \bar{N}^\beta(\mathbf{z}, t) \bar{N}^\eta(\mathbf{w}, t) \times \\ &\quad \bar{N}^\delta(\mathbf{0}, 0) \bar{N}^\psi(\mathbf{0}, 0) N^\gamma(\mathbf{0}, 0) N^\zeta(\mathbf{0}, 0) | 0 \rangle - \langle \theta_{NN}(t) \rangle^2 \\ &\rightarrow Z_{NN\bar{N}\bar{N}} e^{-4M_N t} - Z_{NN}^2 e^{-4M_N t} + Z_{3\pi N\bar{N}} e^{-(2M_N + 3m_\pi)t} + Z_{6\pi} e^{-6m_\pi t} + \dots \\ &\rightarrow Z_{6\pi} e^{-6m_\pi t}. \end{aligned} \quad (76)$$

Therefore, we anticipate finding energy scales of approximately $E_s = 0$, $M_N - \frac{3}{2}m_\pi$ and $2M_N - 3m_\pi$ in

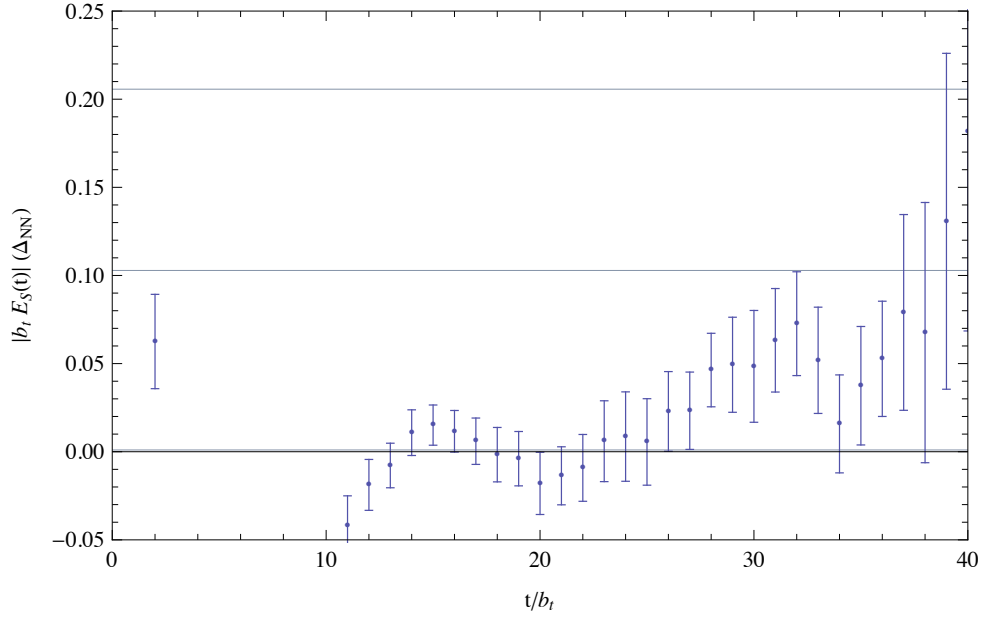


Figure 25: The energy scale of the signal-to-noise ratio, defined in Eq. (74), in the ratio of correlation functions that produces the shift in energy between two interacting protons and two isolated protons, obtained on $20^3 \times 128$ anisotropic clover gauge field configurations [115, 116, 117]. The horizontal lines in the left panel correspond to $E_s = 0$, $M_N - \frac{3}{2}m_\pi$ and $2M_N - 3m_\pi$.

the signal-to-noise ratio on gauge field configurations of infinite temporal extent, see Figure 24. The temporal boundary conditions imposed in the present calculation introduce additional energy scales due to the backward propagating states. Figure 25 shows the energy scale associated with the signal-to-noise ratio for the ratio of correlation functions that provides the energy splitting between two interacting protons and two isolated protons from which the $p \cot \delta(p)$ is extracted, obtained on $20^3 \times 128$ anisotropic clover gauge field configurations [115, 116, 117]. It is clear that the energy scale of the energy splitting is significantly less than for the individual energies, and is consistent with zero throughout much of the Golden Window of time slices. This indicates that the signal-to-noise ratio associated with the energy splitting in the proton-proton sector, and hence the scattering parameters and bound-state energies, are time independent, and therefore do not degrade exponentially with time. This is an exceptionally important result, as it means that the extraction of NN, and more generally, multi-nucleon interactions, does not require an exponentially large number of calculations for each relevant correlation function.

The signal-to-noise ratio in the $\Xi\Xi$ sector is noticeably larger than in the NN and the YN sectors. It is likely that the improved signal-to-noise behavior in the $\Xi\Xi$ sector is due to a reduced overlap of the source onto the multi-meson intermediate states in the variance correlation function compared to purely baryonic intermediate states. Such a reduction is expected based on the fact that the volume occupied by multiple Ξ 's is smaller than that of multiple nucleons, and serves to extend the Golden Window beyond its range in nucleon correlation functions.

As discussed previously, the correlation functions for states with the quantum numbers of the triton (or ${}^3\text{He}$) and $\Xi^0\Xi^0 n$ have been calculated, with well-defined plateaus being observed in the EMPs in both channels. As the largest number of calculations have been performed in the $\Xi^0\Xi^0 n$ channel, the signal-to-noise ratio of its correlation function has been calculated [116]. In Figure 26 we show the energy-scales associated with the signal-to-noise ratios for the $\Xi^0\Xi^0 n$ correlation function as a function of time-slice [116]. In particular, the right-panel shows that the difference of energy-scales between

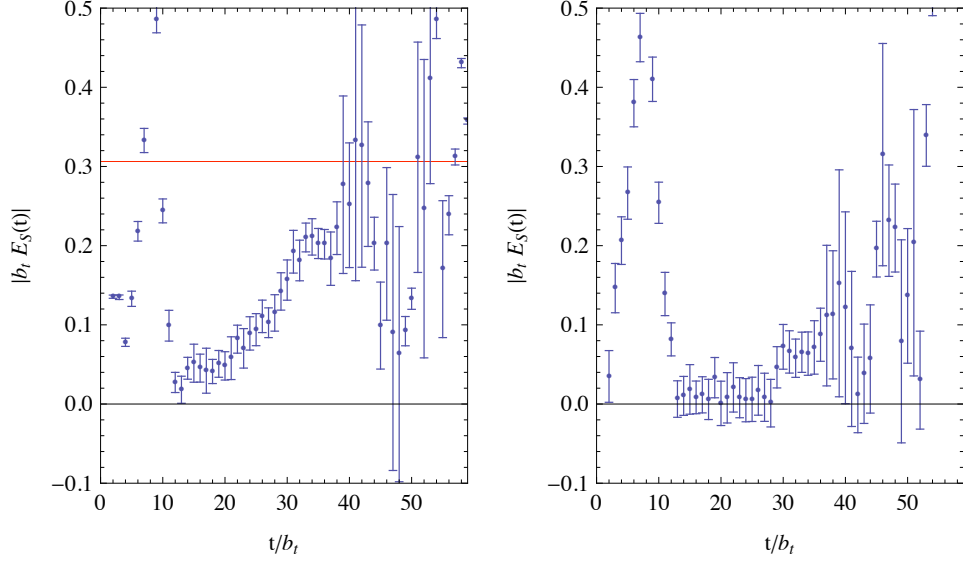


Figure 26: The left panel shows the energy-scales associated with the signal-to-noise ratio for the $\Xi^0 \Xi^0 n$ correlation function [116], as defined in Eq. (74). The horizontal line corresponds to $m_N + 2m_\Xi - 2m_\eta - \frac{5}{2}m_\pi$, the asymptotic energy-scale in a lattice with infinite temporal extent. The right panel shows the difference between the signal-to-noise energy scales of the diagonalized $\Xi^0 \Xi^0 n$ correlation function and that of the nucleon and twice that of the Ξ correlation function.

the three-baryon system and its constituents is consistent with zero within the Golden Window of time-slices. It is clear from this figure that the current computational technology used by NPLQCD would allow for the calculation of systems with $A > 3$ using algorithms that allow for the multi-baryon contractions to be performed in a reasonable amount of computer time.

In Figure 27, the relative uncertainties in the extraction of one-, two- and three-baryon ground state energies obtained in Refs. [115, 116, 117] are shown. It is somewhat remarkable from the numerical standpoint that the relative uncertainty per baryon is essentially independent of baryon number when determined within the Golden Window of time-slices. With the high-statistics calculations performed by the NPLQCD collaboration, an uncertainty of approximately 6 MeV per baryon has been obtained, which is at the threshold for performing meaningful calculations for nuclear physics (once the pion mass is reduced to its physical value).

It is clear that the Golden Window of time-slices that has been uncovered in Refs. [115, 116, 117], which provides a way to evade the need for exponentially large computational resources to calculate multi-baryon systems, requires careful source and sink optimization. This involves two considerations to make optimal use of available resources:

1. maximal overlap of the interpolating operators onto the baryon states
2. minimum overlap of the interpolating operators onto the mesonic states in the correlation function dictating the variance of the baryon correlation functions

To close this section, we make the comment that it is highly desirable to develop algorithms that explicitly eliminate the exponential degradation of the signal-to-noise ratio in generic correlation functions. While this is an obvious comment to make, such algorithms do not yet exist, however, there have been encouraging developments. It has been shown, by Lüscher and Weisz [139], that a multi-level

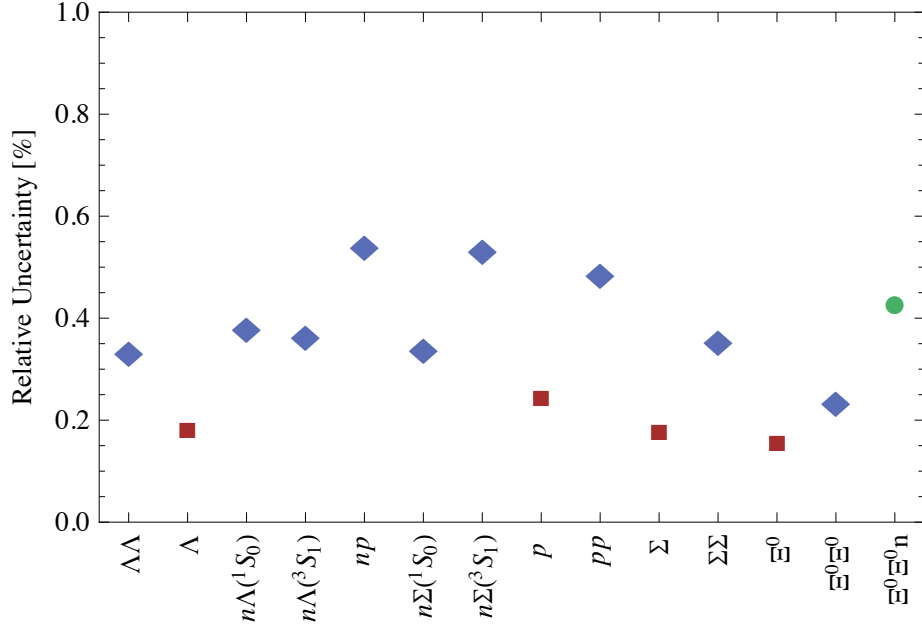


Figure 27: The relative uncertainties in the extraction of one-, two- and three-baryon ground state energies obtained in Refs. [115, 116, 117].

scheme, involving the iterative sequential update of gauge fields and averaging the products of gauge links, leads to large Wilson-loops that have statistical uncertainties that are exponentially smaller than those resulting from the usual method of evaluation (direct evaluation of the Wilson loop on each member of the ensemble of gauge configurations). This multi-level scheme has been applied to the calculation of the Yang-Mills spectrum by inserting projectors into the transfer-matrix that restrict the quantum numbers of the states that can propagate forward in time [140, 141]. Such projections lead to an exponential improvement in the time-dependence of the signal-to-noise ratio. It is conceivable that analogous projections can be developed for $n_f = 2 + 1$ calculations, for instance producing gauge field configurations which do not permit the propagation of single pions, thereby eliminating the long-time correlations in the light-quark propagators, and thereby exponentially reducing the cancellations that occur in forming the correlation functions for one or more baryons. There has also been progress in the calculation of the properties of spin-systems by using cluster-algorithms where the partition functions is split into the sum of contributions that individually do not suffer from the sign problem, e.g. Ref. [142]. However, this algorithm has yet to be transcribed into Lattice QCD calculations.

6 Optimization through the Analysis of Simulated Calculations

Large computational resources are required to perform Lattice QCD calculations, especially of quantities that impact nuclear physics. As such, it is important to simulate the results of Lattice QCD calculations in order to estimate the volumes, lattice spacings and pion masses of calculations that will optimize the physics output with fixed resources. As an example, consider the results of a set of simulated calculations on an ensemble of gauge field configurations with spatial dimensions $L \sim 12.3$ fm at the physical pion mass ($m_\pi L \sim 8.7$). The experimentally determined nucleon-nucleon $^3S_1 - ^3D_1$ coupled-channels scattering amplitude is used to determine the two energy-levels in the finite lattice volume

Table 3: Simulated calculations of the shifts of the two lowest-lying energy levels of two nucleons in a finite lattice volume with spatial extent $L \sim 12.3$ fm generated from the physical 3S_1 scattering amplitude (at the physical values of the light-quark masses) at varying levels of precision. For simplicity, the precision of the two calculated energy levels are taken to be equal.

Precision Level of Energy Shift	Bound State Energy (MeV)	1 st Continuum Level (MeV)
0%	-3.147	4.005
1%	-3.111 ± 0.031	4.015 ± 0.040
5%	-2.95 ± 0.16	4.24 ± 0.20
10%	-2.66 ± 0.31	3.65 ± 0.40

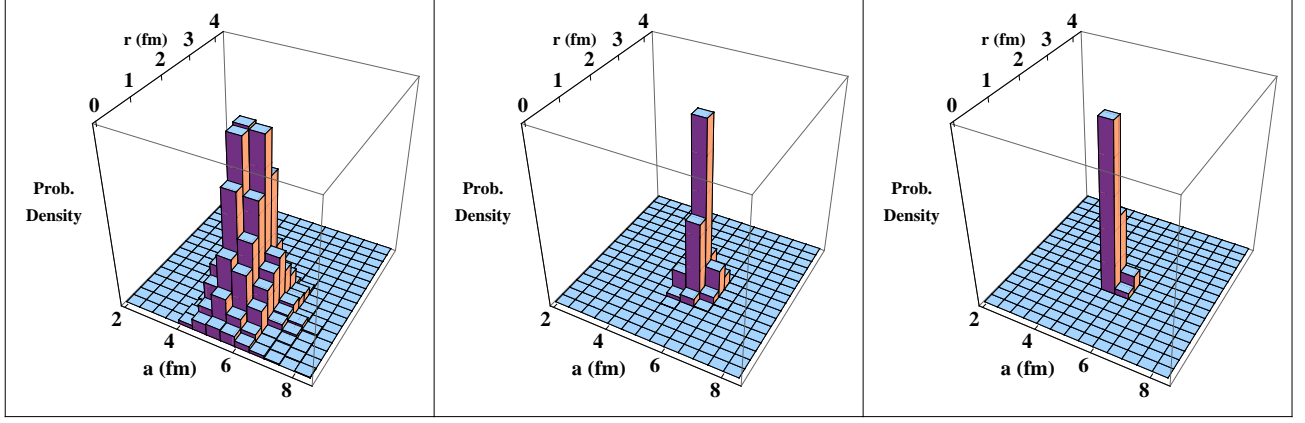


Figure 28: The scattering parameters extracted from Monte-Carlo fitting to the simulated calculations of $p \cot \delta$ shown in Table 3. The left panel corresponds to 10% precision, the middle panel to 5% precision and the right panel to 1% precision.

that are below the inelastic threshold (set by $|\mathbf{p}| < m_\pi/2$) using the Lüscher relation in Eq. (32). In particular, a scattering length of $a^{\text{input}} = 5.425$ fm, an effective range of $r^{\text{input}} = 1.749$ fm, and a nucleon mass of $M_N^{\text{input}} = 939$ MeV are used, which produce a deuteron bound by $B = 2.214$ MeV when d-wave interactions and higher order terms in the effective range expansion are ignored. Simulated results are then generated with 10%, 5% and 1% uncertainties by randomly distributing the centroid of the energy-level by the corresponding amount, and assigning the corresponding uncertainty. The deuteron bound state energy in this finite lattice volume²⁶ is $E_D^{(L)} = -3.147$ MeV, and the lowest lying continuum state appears at $E^{(L)} = +4.005$ MeV. Given the simulated calculations shown in Table 3, the goal is to extract the deuteron binding energy and the scattering parameters at the varying levels of precision.

In order to propagate the correlated uncertainties associated with the extraction of the scattering

²⁶The deuteron becomes more tightly bound in the finite lattice volume due to the exclusion of momentum modes by the periodic boundary conditions imposed in the spatial directions. It is interesting to note that if instead of a volume with periodic boundary conditions, the nucleons were confined with a harmonic oscillator potential, as is common-place in nuclear structure calculations, the deuteron binding energy would be reduced in magnitude due to the positive energy contributions from the potential.

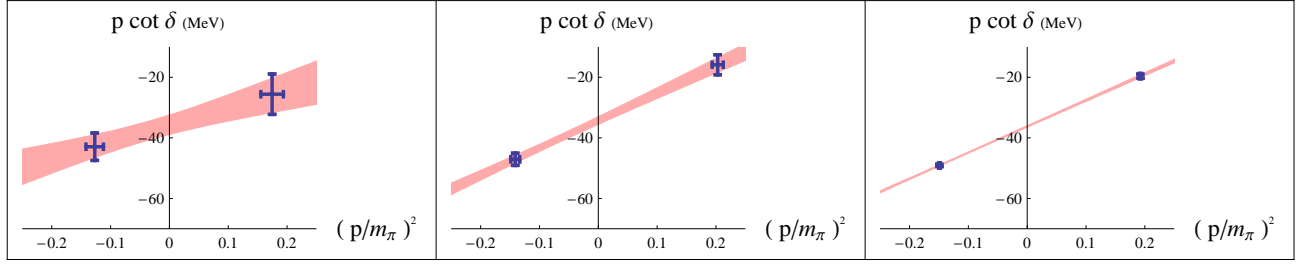


Figure 29: The $1\text{-}\sigma$ determination of the $p \cot \delta$ function (shaded region) extracted from the simulated calculations in Table 3 (shown as points with uncertainties). The left panel corresponds to 10% precision, the middle panel to 5% precision and the right panel to 1% precision.

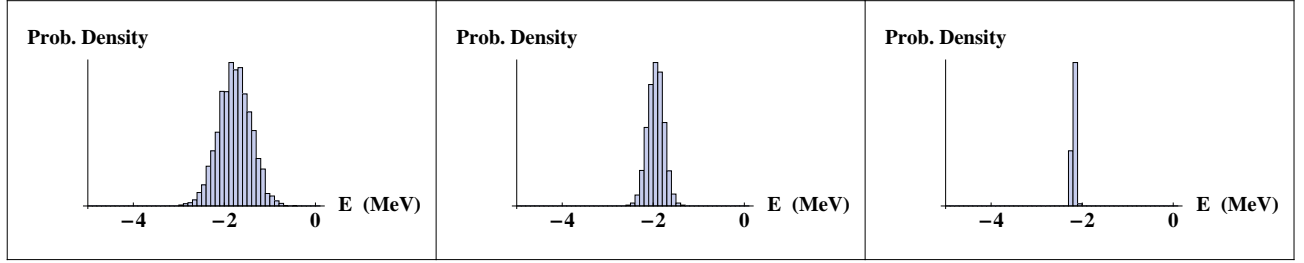


Figure 30: The deuteron binding energy extracted from Monte-Carlo fitting to the simulated calculations in Table 3. The left panel corresponds to 10% precision, the middle panel to 5% precision and the right panel to 1% precision.

parameters, we perform a Monte-Carlo analysis of this simulated set of calculations. For each value of p^2 and of $p \cot \delta$ a value is randomly drawn from a normal-distribution with mean and standard deviation set by the quantity and its uncertainty²⁷. A two-parameter fit is performed in this simplified analysis, terminating the energy expansion of $p \cot \delta$ at the effective range parameter, providing a pair of fit values to the scattering length and effective range, $\{a_i, r_i\}$. The distributions of these extracted pairs are shown in the lego plots in Figure 28. These ensembles of extractions are then used to generate ranges of values of $p \cot \delta$ for any p^2 (using the functional form), from which means and standard deviations can be determined. The results of which are shown in Figure 29. For each pair $\{a_i, r_i\}$, the effective range expression can be used to determine the deuteron binding energy, the distribution of which is shown in Figure 30. The results of the analysis of the simulated calculations are shown in Table 4

A number of conclusions can be drawn from the analysis of simulated calculations:

1. Determining the shifts in the lowest two energy eigenvalues in a lattice with $L \sim 12$ fm with precision exceeding $\sim 10\%$ is sufficient to determine the deuteron binding energy with a precision that exceeds the $5\text{-}\sigma$ -level. For the physical binding energy of the deuteron, 10% uncertainty in the energy shift corresponds to a $\sim 0.01\%$ uncertainty in the total energy. This is approximately an order of magnitude more precise than present calculations.

²⁷ It should be noted that the uncertainties associated with the simulated calculations in Table 3 are uncorrelated (between the p^2 and $p \cot \delta$ for each energy-level). However, this will not be the situation in actual Lattice QCD calculations where $p \cot \delta$ is determined from p^2 using Eq. (32). For this exercise we treat them as independent (which tends to increase calculated uncertainties).

Table 4: Results of the analysis of the simulated calculations in Table 3.

Precision Level	Deuteron Binding Energy (MeV)	Scattering Length (fm)	Effective Range (fm)
0%	−2.214 (input)	5.425 (input)	1.749 (input)
1%	−2.180(35)	5.447(38)	1.737(32)
5%	−1.94(18)	5.77(22)	1.82(16)
10%	−1.77(35)	5.58(51)	1.14(42)

2. The precision of the scattering length extraction is somewhat better than the deuteron binding energy, while that of the effective range is somewhat worse. This is consistent with the fact that the scattering length enters at LO in the momentum expansion of the scattering length, while the effective range enters at NLO.
3. Having calculations on both sides of $p^2 = 0$, combined with the fact that the magnitude of the deuteron binding energy increases as the lattice volume decreases, allows for a much more precise determination of the scattering parameters and deuteron binding energy than would be the case with calculations of the deuteron binding energy alone on two lattice ensembles with different volumes. This is because an interpolation is required to reach the physical deuteron binding energy, as opposed to an extrapolation that would be required for single-level (bound-state) calculations in multiple lattice volumes.
4. A NNLO analysis, including the extraction of the shape-parameter, r_1 requires calculating three energy eigenvalues in one lattice-volume, or calculations on a number of lattice volumes. Given the experimentally observed smallness of the shape parameters contributing to nucleon-nucleon scattering, high-precision calculations of the energy eigenvalues will be required for such an extraction.

7 Other Lattice QCD Efforts in Low-Energy Nuclear Physics

The content of this review is primarily focused on the work of the NPLQCD collaboration, and its efforts to extract the properties and interactions of nuclei from lattice QCD calculations. However, this agenda has been taken up by other collaborations also. As discussed previously, the HALQCD collaboration has performed both quenched and dynamical Lattice QCD calculations of baryon-baryon correlation functions from which non-local, energy-dependent and interpolating operator dependent baryon-baryon potentials are extracted [88, 90]. Unfortunately these potentials contain no more (rigorous) information than the location of the energy-levels in the lattice volume, and the scattering parameters that can be derived using the Lüscher relation. Important work has been recently performed by the PACS-CS collaboration [133]. Exploratory quenched Lattice QCD calculations of the ^3He and ^4He correlation functions strongly suggest that both nuclei are bound for pions with a mass of $m_\pi \sim 800$ MeV.

An exciting development that has taken place during the last couple of years is the exploration of nuclei with $n_f = 1$ Lattice QCD at strong coupling [143, 144]. In this limit there is no Yang-Mills contribution to the action, and instead of integrating out the fermionic fields to leave an integral over the gauge fields that is evaluated by Monte-Carlo, the gauge links are integrated out to leave an integration over the fermion fields which can also be performed in closed-form. The partition function becomes

a weighted sum over configurations of dimers and self-avoiding baryon loops. The nucleon-nucleon potential that is found, is qualitatively consistent with the modern phenomenological nucleon-nucleon potentials. Further, the binding energy of larger nuclei up to ^{12}C derived in this limit, were found to be qualitatively described by the first two terms in the von Weisäcker formula.

An area of Lattice QCD calculations that is peripherally related to multi-nucleon systems, but is having increased overlap with the study of hadronic interactions is the calculation of the excited states of baryons and mesons. At heavier pion masses, where many of the excited states of the nucleon and strange baryons are stable against strong decay, it is somewhat straightforward to calculate their spectrum with lattice QCD. The excited states correspond to exponentially decaying states in the correlation functions created by interpolating operators with the correct quantum numbers. Enormous effort has been put into successfully refining the basis of interpolating operators and developing techniques with which to cleanly separate multiple excited states from the ground-state and other excited states, for example Ref. [58, 145, 146]. The situation becomes vastly more complex as the pion mass approaches the physical value and the resonances become unstable to strong decay. The energy eigenstates in the lattice volume are the baryon ground-state and the scattering states with the same quantum numbers. The excited states correspond to the energies for which the scattering phase-shift is at $\delta_0 = \frac{\pi}{2}$, and the energy interval over which the phase-shift is “near” δ_0 dictates the width. Given that the location of the scattering states in the volume cannot be dictated in the generation of gauge field configurations, calculations must be performed in multiple volumes. Further, given that $m_\pi L \gtrsim 2\pi$ must be satisfied by calculations in order for the wavefunctions to be asymptotic at the boundary of the lattice, the location of multiple excited states in the lattice volume must be precisely determined, e.g. Ref. [147]. This is an exceptionally challenging problem, but progress is being made in extracting the properties of the ρ -meson and the Δ -resonance.

An area that is not Lattice QCD, but which makes use of techniques that were developed for Lattice QCD calculations and impacts low-energy nuclear physics is Lattice Nuclear EFT. Low-energy nuclear structure and reactions are determined in the low-energy EFT using a space-time lattice, and performing the path integral. The conventional power-counting and perturbative expansion that are employed successfully for particle physics observables fail in the nuclear context as nuclei are nonperturbative objects. After many years of development, EFT’s for nuclear physics are reasonably well developed, and recently progress has been made in calculating S-matrix elements in systems involving more than two nucleons by latticizing the EFT’s [136, 148].

8 Resource Requirements and the Next Decade

A number of workshops focusing on the science need for exa-scale computing resources sponsored by the US Department of Energy were held during 2009. One of the workshops, *Forefront Questions in Nuclear Science and the Role of Computing at the Extreme Scale* [149], established the need for exa-scale computing resources in order for the main goals of the field of nuclear physics to be accomplished. One of the major goals of the field that requires exa-scale computing resources is the calculation of nuclear forces from QCD using Lattice QCD, and Figure 31 presents an overview of current estimates of these requirements.

As discussed in a previous review [97], a complete calculation of the nucleon-nucleon scattering amplitude, and the hyperon-nucleon and hyperon-hyperon scattering amplitudes (including multiple lattice spacings, volumes and light quark masses) will require sustained peta-scale resources, as shown in Figure 31. The same is true for the meson-baryon interactions. It is estimated that sustained-sub-peta-scale-year resources are required to perform high-precision calculations of meson-meson scattering-phase shifts, extrapolated to the physical pion mass (in the isospin limit), including the contributions from disconnected diagrams to the iso-singlet $\pi\pi$ channel.

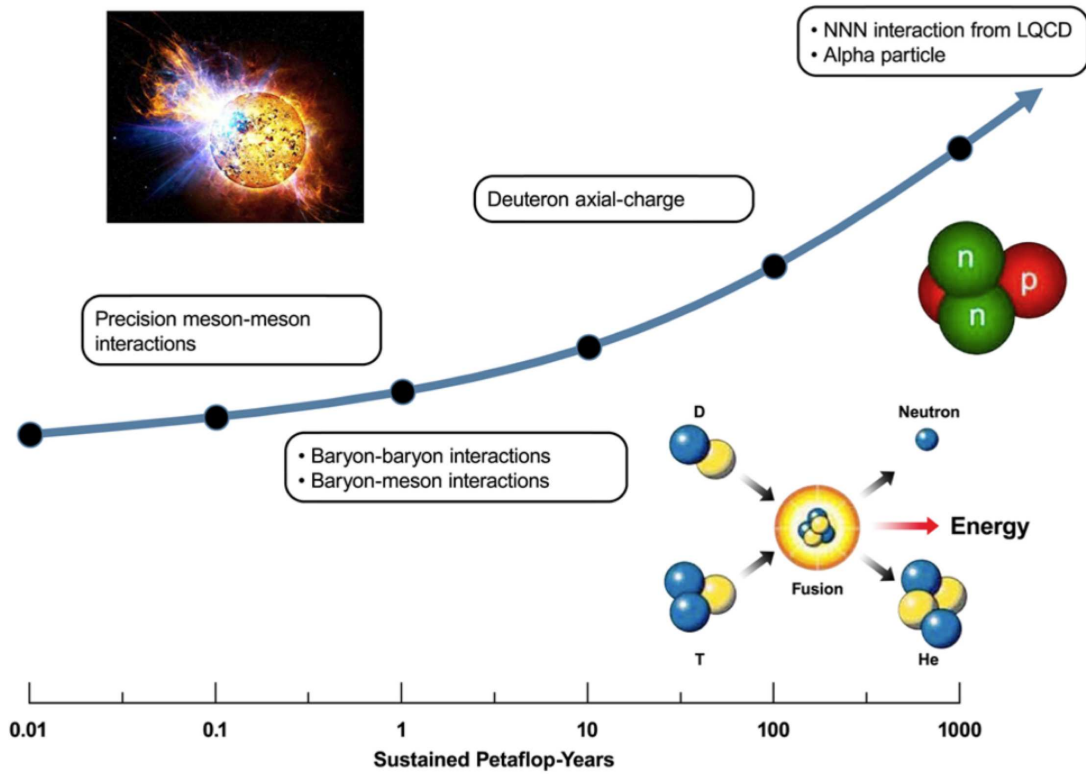


Figure 31: Estimates of the resources required to complete calculations of importance to nuclear physics [149]. Except for the quantities indicated as requiring exa-scale resources, the resource requirements are for calculations performed in the isospin limit and without electroweak interactions.

It is currently estimated that sustained peta-scale resources are required in order to calculate the matrix elements of electroweak operators, such as those determining neutrino-induced breakup of the deuteron, in the few-nucleon sector. Great progress is being made in computing single hadron matrix elements of such operators, such as the isovector axial-current matrix element in the nucleon, g_A [150, 151, 152]. While the extrapolation to the physical pion mass, and to infinite volume remain the subject of discussions in the community, relatively rapid progress is being made. The calculations of matrix elements of operators that receive contributions from disconnected diagrams remain difficult with currently available resources, but will be completed with peta-scale resources. A significant uncertainty in the experimentally determined properties of neutrinos comes from the uncertainties in weak matrix elements between nuclear states. Such uncertainties in few-nucleon systems should be reduced within the next decade with anticipated Lattice QCD calculations, as indicated in Figure 31.

Despite the first Lattice QCD calculations of three- (dynamical [116]) and four-baryon (quenched [133]) systems appearing this year, it is estimated that exa-scale computing resources will be required to extract the nuclear interactions among three-nucleons and determine the spectrum of the α -particle. Given that the three-nucleon interaction is relatively imprecisely known when compared with the two-nucleon interactions, this calculation will have significant impact upon nuclear structure and reaction calculations. The three-baryon interactions between strange and non-strange baryons will be calculable at the same time with the same level of precision with minimal additional resource requirements.

The current discussions regarding exa-scale computing facilities suggests that it may be possible to see such resources deployed sometime around 2018 [149]. Clearly, such resources are required for the calculation of quantities of central importance to the nuclear physics program. During the next decade

the field will develop the ability to perform low-energy strong interaction calculations with quantifiable uncertainty estimation. Lattice QCD will supplement the present ability of the experimental nuclear physics program to determine quantities with certain precision to processes that cannot be accessed experimentally.

9 Conclusion

A central goal of the field of nuclear physics is to establish a framework with which to perform high-precision calculations, with quantifiable uncertainties, of strong-interaction processes occurring under a broad range of conditions. Quantum chromodynamics was established as the underlying theory of the strong interactions during the 1970's, however, nuclear physics is the regime of QCD in which its defining property of asymptotic freedom is hidden by the vacuum and by the phenomenon of confinement. Lattice QCD, in which the QCD path integral is evaluated numerically, is the only known way to perform rigorous QCD calculations of low-energy strong interaction processes. With the research and development into high-performance computing, nuclear physics, quantum field theory, applied mathematics, and numerical algorithms that has taken place over the last few decades, the field of nuclear physics is entering into an era in which Lattice QCD will become a quantitative tool in much the same way that experiments are, but with a different scope and different range of applicability. Rapid progress is currently being made in the calculation of the interactions among nucleons and, more generally, among the low-lying baryons. Present day Lattice QCD calculations are being performed at pion masses larger than the physical pion mass, but as exploratory calculations are now being performed at the physical pion mass, the interactions among baryons will be known from QCD at the physical light-quark masses within the next several years (if computational resources devoted to these calculations continue to increase as they have during the last decade).

Determining the three-body and higher-body interactions among nucleons and hyperons directly from QCD will be a remarkable achievement for Lattice QCD, and will provide crucial input into the calculations of the structure and interactions of light nuclei. During the last year the first calculations of three- and four- nucleon systems were reported. Such calculations are presently difficult, but are primarily limited by the available computational resources and not by conceptual or formal issues. It is anticipated that the three-nucleon interactions will be calculated with high-precision with Lattice QCD during the next decade. Beyond the three-body systems, we expect that some of the properties and interactions of light nuclei will be calculable with Lattice QCD during the same time-period.

The dream of being able to perform reliable calculations of the interactions among multiple nucleons and hyperons, and of the structure and reactions of light-nuclei, directly from QCD is starting to be realized. The path forward is clear, and the next decade will be a truly remarkable period for nuclear physics.

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References

- [1] K. G. Wilson, Phys. Rev. D **10**, 2445 (1974).
- [2] S. C. Pieper, Riv. Nuovo Cim. **031**, 709 (2008) [arXiv:0711.1500 [nucl-th]].
- [3] R. B. Wiringa, V. G. J. Stoks and R. Schiavilla, Phys. Rev. C **51**, 38 (1995) [arXiv:nucl-th/9408016].
- [4] D. Page and S. Reddy, Ann. Rev. Nucl. Part. Sci. **56**, 327 (2006) [arXiv:astro-ph/0608360].
- [5] K. Symanzik, Nucl. Phys. B **226**, 205 (1983).
- [6] R. Gupta, arXiv:hep-lat/9807028.
- [7] B. Sheikholeslami and R. Wohlert, Nucl. Phys. B **259**, 572 (1985).
- [8] R. Frezzotti, P. A. Grassi, S. Sint and P. Weisz [Alpha collaboration], JHEP **0108**, 058 (2001) [arXiv:hep-lat/0101001].
- [9] J. B. Kogut and L. Susskind, Phys. Rev. D **11**, 395 (1975).
- [10] D. B. Kaplan, Phys. Lett. B **288**, 342 (1992) [arXiv:hep-lat/9206013].
- [11] Y. Shamir, Nucl. Phys. B **406**, 90 (1993) [arXiv:hep-lat/9303005].
- [12] V. Furman and Y. Shamir, Nucl. Phys. B **439**, 54 (1995) [arXiv:hep-lat/9405004].
- [13] R. Narayanan and H. Neuberger, Nucl. Phys. B **443**, 305 (1995) [arXiv:hep-th/9411108].
- [14] H. Neuberger, Phys. Lett. B **417**, 141 (1998) [arXiv:hep-lat/9707022].
- [15] P. H. Ginsparg and K. G. Wilson, Phys. Rev. D **25**, 2649 (1982).
- [16] A. Hasenfratz, P. Hasenfratz, F. Niedermayer, D. Hierl and A. Schafer, PoS **LAT2006**, 178 (2006) [arXiv:hep-lat/0610096].
- [17] C. Gattringer, Phys. Rev. D **63**, 114501 (2001) [arXiv:hep-lat/0003005].
- [18] C. Gattringer *et al.* [BGR Collaboration and Bern-Graz-Regensburg Collaboration], Nucl. Phys. B **677**, 3 (2004) [arXiv:hep-lat/0307013].
- [19] P. de Forcrand, PoS **LAT2009**, 010 (2009) [arXiv:1005.0539 [hep-lat]].
- [20] K. Orginos, D. Toussaint and R. L. Sugar [MILC Collaboration], Phys. Rev. D **60**, 054503 (1999) [arXiv:hep-lat/9903032].
- [21] K. Orginos and D. Toussaint [MILC collaboration], Phys. Rev. D **59**, 014501 (1999) [arXiv:hep-lat/9805009].
- [22] Y. Shamir, Phys. Rev. D **75**, 054503 (2007) [arXiv:hep-lat/0607007].
- [23] C. Bernard, M. Golterman and Y. Shamir, Phys. Rev. D **73**, 114511 (2006) [arXiv:hep-lat/0604017].
- [24] C. Bernard, M. Golterman and Y. Shamir, Phys. Rev. D **77**, 074505 (2008) [arXiv:0712.2560 [hep-lat]].

- [25] C. Bernard, M. Golterman, Y. Shamir and S. R. Sharpe, Phys. Rev. D **77**, 114504 (2008) [arXiv:0711.0696 [hep-lat]].
- [26] S. Dürr and C. Hoelbling, Phys. Rev. D **74**, 014513 (2006) [arXiv:hep-lat/0604005].
- [27] S. Dürr and C. Hoelbling, Phys. Rev. D **71**, 054501 (2005) [arXiv:hep-lat/0411022].
- [28] C. Bernard, M. Golterman, Y. Shamir and S. R. Sharpe, Phys. Lett. B **649**, 235 (2007) [arXiv:hep-lat/0603027].
- [29] M. Creutz, PoS **LAT2007**, 007 (2007) [arXiv:0708.1295 [hep-lat]].
- [30] T. Takaishi and P. de Forcrand, Phys. Rev. E **73**, 036706 (2006) [arXiv:hep-lat/0505020].
- [31] S. Duane, A. D. Kennedy, B. J. Pendleton and D. Roweth, Phys. Lett. B **195**, 216 (1987).
- [32] S. A. Gottlieb, W. Liu, D. Toussaint, R. L. Renken and R. L. Sugar, Phys. Rev. D **35**, 2531 (1987).
- [33] M. Lüscher, Comput. Phys. Commun. **165**, 199 (2005) [arXiv:hep-lat/0409106].
- [34] W. Kamleh and M. J. Peardon [TrinLat Collaboration], PoS **LAT2005**, 106 (2006).
- [35] M. Hasenbusch, Phys. Lett. B **519**, 177 (2001) [arXiv:hep-lat/0107019].
- [36] D. H. Weingarten and J. C. Sexton, Nucl. Phys. Proc. Suppl. **26**, 613 (1992).
- [37] M. J. Peardon and J. Sexton [TrinLat Collaboration], Nucl. Phys. Proc. Suppl. **119**, 985 (2003) [arXiv:hep-lat/0209037].
- [38] M. A. Clark and A. D. Kennedy, Phys. Rev. Lett. **98**, 051601 (2007) [arXiv:hep-lat/0608015].
- [39] C. Jung, arXiv:1001.0941 [hep-lat].
- [40] C. W. Bernard *et al.*, Phys. Rev. D **64**, 054506 (2001) [arXiv:hep-lat/0104002].
- [41] J. W. Chen, D. O’Connell and A. Walker-Loud, JHEP **0904**, 090 (2009) [arXiv:0706.0035 [hep-lat]].
- [42] J. W. Chen, D. O’Connell, R. S. Van de Water and A. Walker-Loud, Phys. Rev. D **73**, 074510 (2006) [arXiv:hep-lat/0510024].
- [43] J. W. Chen, D. O’Connell and A. Walker-Loud, Phys. Rev. D **75**, 054501 (2007) [arXiv:hep-lat/0611003].
- [44] R. G. Edwards *et al.* [LHPC Collaboration], PoS **LAT2006**, 195 (2006).
- [45] D. B. Renner *et al.* [LHPC Collaboration], PoS **LAT2007**, 160 (2007) [arXiv:0710.1373 [hep-lat]].
- [46] Ph. Hagler *et al.* [LHPC Collaborations], Phys. Rev. D **77**, 094502 (2008) [arXiv:0705.4295 [hep-lat]].
- [47] R. G. Edwards *et al.*, PoS **LAT2006**, 121 (2006) [arXiv:hep-lat/0610007].
- [48] R. G. Edwards *et al.* [LHPC Collaboration], Phys. Rev. Lett. **96**, 052001 (2006) [arXiv:hep-lat/0510062].
- [49] D. Toussaint and K. Orginos [MILC Collaboration], Nucl. Phys. Proc. Suppl. **73**, 909 (1999) [arXiv:hep-lat/9809148].
- [50] K. Orginos, R. Sugar and D. Toussaint, Nucl. Phys. Proc. Suppl. **83**, 878 (2000) [arXiv:hep-lat/9909087].
- [51] W. J. Lee and S. R. Sharpe, Phys. Rev. D **60**, 114503 (1999) [arXiv:hep-lat/9905023].
- [52] D. B. Renner *et al.* [LHP Collaboration], Nucl. Phys. Proc. Suppl. **140**, 255 (2005) [arXiv:hep-lat/0409130].
- [53] R. G. Edwards *et al.* [LHPC Collaboration], PoS **LAT2005**, 056 (2006) [arXiv:hep-lat/0509185].
- [54] M. Okamoto *et al.* [CP-PACS Collaboration], Phys. Rev. D **65**, 094508 (2002) [arXiv:hep-lat/0112020].
- [55] P. Chen, Phys. Rev. D **64**, 034509 (2001) [arXiv:hep-lat/0006019].
- [56] C. Morningstar and M. J. Peardon, Phys. Rev. D **69**, 054501 (2004) [arXiv:hep-lat/0311018].

- [57] J. J. Dudek, R. G. Edwards, M. J. Peardon, D. G. Richards and C. E. Thomas, Phys. Rev. Lett. **103**, 262001 (2009) [arXiv:0909.0200 [hep-ph]].
- [58] J. M. Bulava *et al.*, Phys. Rev. D **79**, 034505 (2009) [arXiv:0901.0027 [hep-lat]].
- [59] H. W. Lin *et al.* [Hadron Spectrum Collaboration], Phys. Rev. D **79**, 034502 (2009) [arXiv:0810.3588 [hep-lat]].
- [60] R. G. Edwards, B. Joo and H. W. Lin, Phys. Rev. D **78**, 054501 (2008) [arXiv:0803.3960 [hep-lat]].
- [61] S. Syritsyn and J. W. Negele, PoS **LAT2007**, 078 (2007) [arXiv:0710.0425 [hep-lat]].
- [62] M. Lüscher, Commun. Math. Phys. **104**, 177 (1986).
- [63] M. Lüscher and U. Wolff, Nucl. Phys. B **339**, 222 (1990).
- [64] T. A. DeGrand and D. Toussaint, *Singapore, Singapore: World Scientific (1990) 750 p*
- [65] C. Michael, Nucl. Phys. B **259**, 58 (1985).
- [66] J. Foley, A. O’Cais, M. Peardon and S. M. Ryan, Phys. Rev. D **75** (2007) 094503 [arXiv:hep-lat/0702010].
- [67] S. Basak *et al.*, Phys. Rev. D **76** (2007) 074504 [arXiv:0709.0008 [hep-lat]].
- [68] B. Blossier, M. Della Morte, G. von Hippel, T. Mendes and R. Sommer, JHEP **0904**, 094 (2009) [arXiv:0902.1265 [hep-lat]].
- [69] J. Juge, Presentation at the USQCD All-Hands meeting at the Jefferson Laboratory, April 2008.
- [70] G. T. Fleming, arXiv:hep-lat/0403023.
- [71] F.B. Hildebrand, “Introduction to Numerical Analysis”, *2nd ed* Dover, 1987.
- [72] G. R. de Prony Journal de l’cole Polytechnique, volume 1, cahier 22, 24-76 (1795).
- [73] H. W. Lin and S. D. Cohen, arXiv:0709.1902 [hep-lat].
- [74] S. R. Beane *et al.*, Phys. Rev. D **79**, 114502 (2009) [arXiv:0903.2990 [hep-lat]].
- [75] G. T. Fleming, S. D. Cohen, H. W. Lin and V. Pereyra, PoS **LAT2007**, 096 (2007).
- [76] L. Maiani and M. Testa, Phys. Lett. B **245**, 585 (1990).
- [77] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).
- [78] M. Lüscher, Commun. Math. Phys. **105**, 153 (1986).
- [79] M. Lüscher, Nucl. Phys. B **354**, 531 (1991).
- [80] J.E. Mandula, G. Zweig and J. Govaerts, *Nucl. Phys.* **B228**, 91 (1983).
- [81] H. W. Hamber, E. Marinari, G. Parisi and C. Rebbi, Nucl. Phys. B **225**, 475 (1983).
- [82] S. R. Beane, P. F. Bedaque, A. Parreño and M. J. Savage, Phys. Lett. B **585**, 106 (2004) [arXiv:hep-lat/0312004].
- [83] S. Sasaki and T. Yamazaki, Phys. Rev. D **74**, 114507 (2006) [arXiv:hep-lat/0610081].
- [84] S. Aoki *et al.* [CP-PACS Collaboration], Nucl. Phys. Proc. Suppl. **140**, 305 (2005) [arXiv:hep-lat/0409063].
- [85] S. Aoki *et al.* [CP-PACS Collaboration], Phys. Rev. D **71**, 094504 (2005) [arXiv:hep-lat/0503025].
- [86] S. Aoki, T. Hatsuda and N. Ishii, Prog. Theor. Phys. **123**, 89 (2010) [arXiv:0909.5585 [hep-lat]].
- [87] W. Detmold, K. Orginos and M. J. Savage, Phys. Rev. D **76**, 114503 (2007) [arXiv:hep-lat/0703009].
- [88] N. Ishii, S. Aoki and T. Hatsuda, Phys. Rev. Lett. **99**, 022001 (2007) [arXiv:nucl-th/0611096].
- [89] S. Aoki, lectures presented at the 13th Taiwan Nuclear Physics Summer School, 2009. <http://phys.cts.ntu.edu.tw/nuclear/2009/Aoki3.pdf>.
- [90] H. Nemura, N. Ishii, S. Aoki and T. Hatsuda, Phys. Lett. B **673**, 136 (2009) [arXiv:0806.1094 [nucl-th]].

- [91] S. Weinberg, Phys. Rev. Lett. **17**, 616 (1966).
- [92] G. Colangelo, J. Gasser and H. Leutwyler, Nucl. Phys. B **603**, 125 (2001) [arXiv:hep-ph/0103088].
- [93] H. Leutwyler, PoS C **CONFINEMENT8**, 068 (2008) [arXiv:0812.4165 [hep-ph]].
- [94] S. M. Roy, Phys. Lett. B **36**, 353 (1971).
- [95] S. R. Beane, T. C. Luu, K. Orginos, A. Parreno, M. J. Savage, A. Torok and A. Walker-Loud, Phys. Rev. D **77**, 014505 (2008) [arXiv:0706.3026 [hep-lat]].
- [96] X. Feng, K. Jansen and D. B. Renner, Phys. Lett. B **684**, 268 (2010) [arXiv:0909.3255 [hep-lat]].
- [97] S. R. Beane, K. Orginos and M. J. Savage, Int. J. Mod. Phys. E **17**, 1157 (2008) [arXiv:0805.4629 [hep-lat]].
- [98] K. Sasaki, N. Ishizuka, T. Yamazaki and M. Oka [PACS-CS Collaboration], PoS **LAT2009**, 098 (2009) [arXiv:0911.0228 [hep-lat]].
- [99] C. Miao, X. i. Du, G. w. Meng and C. Liu, Phys. Lett. B **595**, 400 (2004) [arXiv:hep-lat/0403028].
- [100] J. Nagata, S. Muroya and A. Nakamura, Phys. Rev. C **80**, 045203 (2009) [arXiv:0812.1753 [hep-lat]].
- [101] D. B. Kaplan and A. E. Nelson, preprint HUTP-86/A023; Phys. Lett. B **175** (1986) 57; Phys. Lett. B **192**, 193 (1987); Nucl. Phys. A **479**, 273 (1988); Nucl. Phys. A **479**, 285 (1988);
- [102] M. Lu, M. B. Wise and M. J. Savage, Phys. Lett. B **337**, 133 (1994) [arXiv:hep-ph/9407260].
- [103] E. E. Jenkins and A. V. Manohar, “Baryon chiral perturbation theory using a heavy fermion Lagrangian,” Phys. Lett. B **255**, 558 (1991).
- [104] A. Torok *et al.*, arXiv:0907.1913 [hep-lat].
- [105] Y. R. Liu and S. L. Zhu, Phys. Rev. D **75**, 034003 (2007) [arXiv:hep-ph/0607100].
- [106] Y. R. Liu and S. L. Zhu, Eur. Phys. J. C **52**, 177 (2007) [arXiv:hep-ph/0702246].
- [107] M. Mai, P. C. Bruns, B. Kubis and U. G. Meissner, Phys. Rev. D **80**, 094006 (2009) [arXiv:0905.2810 [hep-ph]].
- [108] S. R. Beane and M. J. Savage, Nucl. Phys. A **713**, 148 (2003) [arXiv:hep-ph/0206113].
- [109] S. R. Beane and M. J. Savage, Nucl. Phys. A **717**, 91 (2003) [arXiv:nucl-th/0208021].
- [110] E. Epelbaum, U. G. Meissner and W. Gloeckle, Nucl. Phys. A **714**, 535 (2003) [arXiv:nucl-th/0207089].
- [111] M. Fukugita, Y. Kuramashi, H. Mino, M. Okawa and A. Ukawa, Phys. Rev. Lett. **73**, 2176 (1994) [arXiv:hep-lat/9407012].
- [112] M. Fukugita, Y. Kuramashi, M. Okawa, H. Mino and A. Ukawa, Phys. Rev. D **52**, 3003 (1995) [arXiv:hep-lat/9501024].
- [113] S. R. Beane, P. F. Bedaque, K. Orginos and M. J. Savage, Phys. Rev. Lett. **97**, 012001 (2006) [arXiv:hep-lat/0602010].
- [114] S. R. Beane, P. F. Bedaque, T. C. Luu, K. Orginos, E. Pallante, A. Parreno and M. J. Savage [NPLQCD Collaboration], Nucl. Phys. A **794**, 62 (2007) [arXiv:hep-lat/0612026].
- [115] S. R. Beane *et al.*, Phys. Rev. D **79**, 114502 (2009) [arXiv:0903.2990 [hep-lat]].
- [116] S. R. Beane *et al.*, Phys. Rev. D **80**, 074501 (2009) [arXiv:0905.0466 [hep-lat]].
- [117] S. R. Beane *et al.*, arXiv:0912.4243 [hep-lat].
- [118] S. Aoki, T. Hatsuda and N. Ishii, Comput. Sci. Dis. **1**, 015009 (2008) [arXiv:0805.2462 [hep-ph]].
- [119] S. R. Beane, W. Detmold and M. J. Savage, Phys. Rev. D **76**, 074507 (2007) [arXiv:0707.1670 [hep-lat]].
- [120] S. Tan, arXiv:0709.2530 [cond-mat.stat-mech].

- [121] W. Detmold and M. J. Savage, Phys. Rev. D **77**, 057502 (2008) [arXiv:0801.0763 [hep-lat]].
- [122] T. Luu, PoS **LATTICE2008**, 246 (2008) [arXiv:0810.2331 [hep-lat]].
- [123] W. Detmold, K. Orginos, M. J. Savage and A. Walker-Loud, Phys. Rev. D **78**, 054514 (2008) [arXiv:0807.1856 [hep-lat]].
- [124] W. Detmold, M. J. Savage, A. Torok, S. R. Beane, T. C. Luu, K. Orginos and A. Parreno, Phys. Rev. D **78**, 014507 (2008) [arXiv:0803.2728 [hep-lat]].
- [125] S. R. Beane, W. Detmold, T. C. Luu, K. Orginos, M. J. Savage and A. Torok, Phys. Rev. Lett. **100**, 082004 (2008) [arXiv:0710.1827 [hep-lat]].
- [126] David H. Bailey, Yozo Hida, Xiaoye S. Li and Brandon Thompson, "ARPREC: An Arbitrary Precision Computation Package," manuscript, Sept 2002; LBNL-53651. Available from <http://crd.lbl.gov/~dhbailey/mpdist/>.
- [127] B. Smigielski and J. Wasem, Phys. Rev. D **79**, 054506 (2009) [arXiv:0811.4392 [hep-lat]].
- [128] B. Smigielski, *private communication*.
- [129] W. Detmold and M. J. Savage, arXiv:1001.2768 [hep-lat].
- [130] D. T. Son and M. A. Stephanov, Phys. Rev. Lett. **86**, 592 (2001) [arXiv:hep-ph/0005225].
- [131] T. Matsui and H. Satz, Phys. Lett. B **178**, 416 (1986).
- [132] W. Detmold and M. J. Savage, Phys. Rev. Lett. **102**, 032004 (2009) [arXiv:0809.0892 [hep-lat]].
- [133] T. Yamazaki, Y. Kuramashi, A. Ukawa (PACS-CS Collaboration), arXiv:0912.1383 [hep-lat].
- [134] S. Kreuzer and H. W. Hammer, Eur. Phys. J. A **43**, 229 (2010) [arXiv:0910.2191 [nucl-th]].
- [135] S. Kreuzer, talk presented at the INT workshop on *Finite-Volume Effects in Few-Body Systems*, April 2010, Seattle, Washington. http://www.int.washington.edu/PROGRAMS/10-1_wkshp.html
- [136] E. Epelbaum, H. Krebs, D. Lee and U. G. Meissner, arXiv:1003.5697 [nucl-th].
- [137] D. Lee, *Private communication* during the INT workshop on *Finite-Volume Effects in Few-Body Systems*, April 2010, Seattle, Washington. http://www.int.washington.edu/PROGRAMS/10-1_wkshp.html
- [138] G. P. Lepage, "The Analysis Of Algorithms For Lattice Field Theory," Invited lectures given at TASI'89 Summer School, Boulder, CO, Jun 4-30, 1989. Published in Boulder ASI 1989:97-120 (QCD161:T45:1989).
- [139] M. Luscher and P. Weisz, JHEP **0109**, 010 (2001) [arXiv:hep-lat/0108014].
- [140] M. Della Morte and L. Giusti, Comput. Phys. Commun. **180**, 819 (2009) [arXiv:0806.2601 [hep-lat]].
- [141] M. Della Morte and L. Giusti, PoS **LATTICE2009**, 029 (2009) [arXiv:0910.2455 [hep-lat]].
- [142] S. Chandrasekharan, Nucl. Phys. Proc. Suppl. **83**, 774 (2000) [arXiv:hep-lat/9909007].
- [143] P. de Forcrand and M. Fromm, Phys. Rev. Lett. **104**, 112005 (2010) [arXiv:0907.1915 [hep-lat]].
- [144] M. Fromm and P. de Forcrand, arXiv:0912.2524 [hep-lat].
- [145] M. S. Mahbub, A. O. Cais, W. Kamleh, D. B. Leinweber and A. G. Williams, arXiv:1004.5455 [hep-lat].
- [146] C. Gatttringer, C. Hagen, C. B. Lang, M. Limmer, D. Mohler and A. Schafer, Phys. Rev. D **79**, 054501 (2009) [arXiv:0812.1681 [hep-lat]].
- [147] M. Gockeler, R. Horsley, Y. Nakamura, D. Pleiter, P. E. L. Rakow, G. Schierholz and J. Zanotti [QCDSF Collaboration], PoS **LATTICE2008**, 136 (2008) [arXiv:0810.5337 [hep-lat]].
- [148] D. Lee, Prog. Part. Nucl. Phys. **63**, 117 (2009) [arXiv:0804.3501 [nucl-th]].

- [149] Scientific Grand Challenges: Forefront Questions in Nuclear Science and the Role of Computing at the Extreme Scale. A workshop sponsored by the Office of Nuclear Physics and the Office of Advanced Scientific Computing Research, held in January 2009. The report is available from <http://extremecomputing.labworks.org/nuclearphysics/report.stm>
- [150] A. A. Khan *et al.*, Phys. Rev. D **74**, 094508 (2006) [arXiv:hep-lat/0603028].
- [151] J. D. Bratt *et al.* [LHPC Collaboration], arXiv:1001.3620 [hep-lat].
- [152] T. Yamazaki *et al.*, Phys. Rev. D **79**, 114505 (2009) [arXiv:0904.2039 [hep-lat]].